31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms

AofA 2020, June 15–19, 2020, Klagenfurt, Austria (Virtual Conference)

Edited by

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ACM Classification 2012
Mathematics of computing; Theory of computation; Computing methodologies

ISBN 978-3-95977-147-4

Published online and open access by
Schloss Dagstuhl – Leibniz-Zentrum für Informatik GmbH, Dagstuhl Publishing, Saarbrücken/Wadern, Germany. Online available at https://www.dagstuhl.de/dagpub/978-3-95977-147-4.

Publication date
June, 2020

Bibliographic information published by the Deutsche Nationalbibliothek
The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at https://portal.dnb.de.

Digital Object Identifier: 10.4230/LIPIcs.AofA.2020.0

LIPIcs – Leibniz International Proceedings in Informatics

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ISSN 1868-8969

https://www.dagstuhl.de/lipics

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Preface

The 31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020) was planned to be held in Klagenfurt, Austria, June 15–19, 2020. Due to the Coronavirus outbreak the conference had to be shifted to an online conference.

Analysis of algorithms is a scientific basis for computation, providing a link between abstract algorithms and the performance characteristics of their implementations in the real world. The general effort to predict precisely the performance of algorithms has come to involve research in analytic combinatorics, the analysis of random discrete structures, asymptotic analysis, exact and limiting distributions, and other fields of inquiry in computer science, probability theory, and enumerative combinatorics. See `http://aofa.cs.purdue.edu/`.

The Call for Papers invited papers in

- analytic algorithmics and combinatorics,
- probabilistic analysis of algorithms, and
- randomized algorithms.

We also welcomed papers addressing problems such as: combinatorial algorithms, string searching and pattern matching, sublinear algorithms on massive data sets, network algorithms, graph algorithms, caching and memory hierarchies, indexing, data mining, data compression, coding and information theory, and computational finance. Papers were also welcomed that address bridges to research in related fields such as statistical physics, computational biology, computational geometry, and simulation.

The present issue collects 25 contributions to the AofA 2020 conference that have been refereed and selected by the Program Committee.

The planned invited speakers were

- Wojciech Szpankowski (Flajolet Lecturer), Purdue University, USA,
- Mireille Bousquet-Mélou, Université de Bordeaux, France,
- James A. Fill, The Johns Hopkins University, Baltimore, USA,
- Malwina Luczak, University of Melbourne, Australia,
- Andrew Rechnitzer, University of British Columbia, Canada.

We acknowledge the financial support by the University of Klagenfurt.

Michael Drmota and Clemens Heuberger,
on behalf of the Program Committee

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On Lattice Paths with Marked Patterns: Generating Functions and Multivariate Gaussian Distribution

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Abstract

In this article, we analyse the joint distribution of some given set of patterns in fundamental combinatorial structures such as words and random walks (directed lattice paths on $\mathbb{Z}^2$). Our method relies on a vectorial generalization of the classical kernel method, and on a matricial generalization of the autocorrelation polynomial (thus extending the univariate case of Guibas and Odlyzko). This gives access to the multivariate generating functions, for walks, meanders (walks constrained to be above the x-axis), and excursions (meanders constrained to end on the x-axis). We then demonstrate the power of our methods by obtaining closed-form expressions for an infinite family of models, in terms of simple combinatorial quantities. Finally, we prove that the joint distribution of the patterns in walks/bridges/excursions/meanders satisfies a multivariate Gaussian limit law.

2012 ACM Subject Classification Mathematics of computing → Generating functions; Mathematics of computing → Distribution functions; Theory of computation → Random walks and Markov chains; Theory of computation → Grammars and context-free languages

Keywords and phrases Lattice path, Dyck path, Motzkin path, generating function, algebraic function, kernel method, context-free grammar, multivariate Gaussian distribution

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.1

Funding *Andrei Asinowski*: supported by the Austrian Science Fund (FWF), in the framework of the project *Analytic Combinatorics: Digits, Automata and Trees* (P 28466-N35).

Acknowledgements We thank the referees for their feedback.

1 Definitions and notations for directed lattice paths

Let $\mathcal{S}$, the *set of steps* (or *jumps*), be some finite subset of $\mathbb{Z}$ that contains at least one negative and at least one positive number. A *lattice path with steps from* $\mathcal{S}$ is a finite word $w = (s_1, s_2, \ldots, s_n)$ in which all letters belong to $\mathcal{S}$, visualized as a directed polygonal line in the plane, which starts in the origin and is formed by successive appending of vectors $(1, s_1), (1, s_2), \ldots, (1, s_n)$. The n letters that form the path $w = (s_1, s_2, \ldots, s_n)$ are referred to as its *steps*. The *length* of w, to be denoted by $\ell(w)$, is the number of steps in w. The *final altitude* of w, to be denoted by $h(w)$, is the sum of all steps in w, that is $s_1 + s_2 + \ldots + s_n$. Visually, $\ell(w)$ and $h(w)$ are the x- and the y-coordinates of the point where w terminates. One considers four classes of paths: a *walk* is any path as described above; a *bridge* is a path that terminates at the x-axis; a *meander* is a path that stays (weakly) above the x-axis; an *excursion* is a path that stays (weakly) above the x-axis and terminates at the x-axis.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
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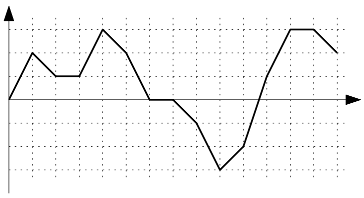
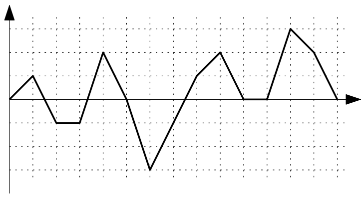
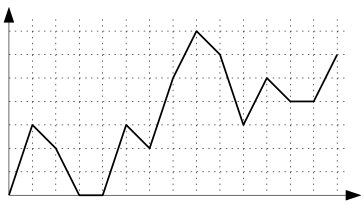
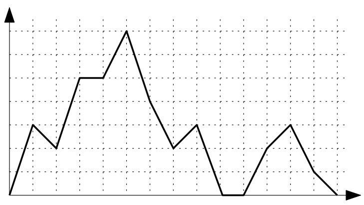
Table 1 For the four types of paths (walks, bridges, meanders, excursions) and for any set of steps encoded by $S(u)$, we give the corresponding generating function marking a set of patterns $p_1, \dots, p_m$. The formulas involve the e small roots u_i (i.e. $u_i(t) \sim 0$ for $t \sim 0$) of the kernel $K(t,u) := (1 - tS(u))\Delta + \Delta'$, where Δ and Δ' are determinants related to the correlation matrix of the patterns. (See Theorems 4, 10, and 12.)

	ending anywhere	ending at 0
on $\mathbb{Z}$	 walks $W(t,u) = \dfrac{\Delta(t,u)}{K(t,u)}$	 bridges $B(t) = -\sum_{i=1}^{e} \dfrac{u_i'}{u_i} \dfrac{\Delta(t,u_i)}{K_t(t,u_i)}$
on $\mathbb{N}$	 meanders $M(t,u) = \dfrac{\Delta(t,u)}{u^e K(t,u)} \prod_{i=1}^{e} (u - u_i(t))$	 excursions $E(t) = \dfrac{(-1)^{e+1}}{t} \prod_{i=1}^{e} u_i(t)$

For each of these classes (in the simpler case of no pattern constraint), Banderier and Flajolet [6] gave general expressions for the corresponding generating functions and the asymptotics of their coefficients. A unified study of lattice paths with **a single forbidden pattern** was recently started by Asinowski, Bacher, Banderier, and Gittenberger [1]: for any fixed path p (a "pattern") they give the generating function and the asymptotics for paths that avoid p as a consecutive string. Moreover, they initiated the more general analysis of **marking a pattern**: here, one considers a generating function with an extra variable v which encodes the number of occurrences of the pattern p in the path. Setting $v = 0$ gives the generating function for walks that avoid p. In this article, we further generalize this work to the case where **several patterns** are marked. The situation is more challenging: more correlations create more obstacles; however, we shall see that one can still derive closed-form expressions in terms of natural combinatorial quantities!

Throughout our article, in the generating functions, the variable t corresponds to the length of a path, and the variable u to its final altitude. $S(u)$ is the *step polynomial* of the set of steps $\mathcal{S}$, defined by

$$S(u) := \sum_{s \in \mathcal{S}} u^s.$$

The set of forbidden/marked patterns will be denoted by $\mathcal{P} = \{p_1, \dots, p_m\}$.

2 Generating functions for walks and bridges with marked patterns

For the case of a single marked pattern p (see e.g. [1, Thm. 7.1]), the trivariate generating function of walks is

$$W(t,u,v) = \frac{v+(1-v)R}{(1-tS)\big(v+(1-v)R\big)+(1-v)t^{\ell(p)}u^{h(p)}}, \tag{1}$$

where t, u, v are the variables as explained in Section 1; $\ell(p)$ and $h(p)$ are the length and the final altitude of the pattern p; and $R = R(t,u)$ is the autocorrelation polynomial that encodes the overlaps of p with itself – see the definition below. The specialization $v = 0$ gives $W(t,u,0) = R/\big((1-tS)R + t^{\ell(p)}u^{h(p)}\big)$, the generating function of walks that avoid p; and $v = 1$ gives $W(t,u,1) = 1/(1-tS)$ – as expected, since it enumerates all the walks over $\mathcal{S}$.

In this work, we consider the more general case of marking several patterns. To this end, let $\mathcal{S}$ be a set of steps, and let $\mathcal{P} = \{p_1, p_2, \dots, p_m\}$ be a set of patterns (that is, fixed words over $\mathcal{S}$). In what follows, we assume that $\mathcal{P}$ is a *reduced system*, that is, the words $p_1, p_2, \dots, p_m$ do not contain each other (where the inclusion is understood as that of strings, for example $\mathsf{ab} \subset \mathsf{abcd}$ and $\mathsf{bc} \subset \mathsf{abcd}$ but $\mathsf{ac} \not\subset \mathsf{abcd}$).

A central role in our approach is played by the notion of *mutual correlation*, a way to formalize how patterns overlap with each other. Given two patterns p_i and p_j, an *overlap* of p_i and p_j is a non-empty string that occurs as a suffix in p_i and as a prefix in p_j. Let $\mathcal{O}_{i,j}$ be the set of all overlaps of p_i and p_j. Further, let $\mathcal{C}_{i,j}$ be the set of words obtained from p_j by erasing all the of overlaps p_i and p_j (as prefixes of p_j). More formally, this leads to the following definition.

▶ **Definition 1** (Mutual correlation polynomials). *The mutual correlation sets are defined as*

$$\mathcal{C}_{i,j} = \{q\colon\ \exists q', q''(q'' \neq \epsilon)\colon\ p_i = q'.q'', p_j = q''.q\}. \tag{2}$$

Accordingly, the ***mutual correlation polynomials*** *are defined as*

$$C_{i,j}(t,u) = \sum_{q \in \mathcal{C}_{i,j}} t^{\ell(q)}u^{h(q)}. \tag{3}$$

In particular, for $i = j$, $C_{i,i}(t,u)$ is the *autocorrelation polynomial* introduced in the case of one single pattern by Schützenberger [38] for prefix codes and by Guibas and Odlyzko [27] in the context of text searching and string overlaps, see also [25, Formula (8.81)] for a first generalization.

▶ **Example 2.** Let $p_1 = \mathsf{aaba}$, $p_2 = \mathsf{abab}$. Then we have

- $\mathcal{O}_{1,1} = \{\mathsf{aaba}, \mathsf{a}\}$, $\mathcal{C}_{1,1} = \{\epsilon, \mathsf{aba}\}$, $C_{1,1} = 1 + t^3u^{2a+b}$;
- $\mathcal{O}_{1,2} = \{\mathsf{aba}, \mathsf{a}\}$, $\mathcal{C}_{1,2} = \{\mathsf{b}, \mathsf{bab}\}$, $C_{1,2} = tu^b + t^3u^{a+2b}$;
- $\mathcal{O}_{2,1} = \mathcal{C}_{2,1} = \varnothing$, $C_{2,1} = 0$;
- $\mathcal{O}_{2,2} = \{\mathsf{abab}, \mathsf{ab}\}$, $\mathcal{C}_{2,2} = \{\epsilon, \mathsf{ab}\}$, $C_{2,2} = 1 + t^2u^{a+b}$.

Let $W = W(t, u, v_1, \dots, v_m)$ be the generating function for the walks, where each occurrence of the pattern p_i $(i = 1, \dots, m)$ is marked by the variable v_i. That is, the coefficient of $t^\alpha u^\beta v_1^{\gamma_1} \dots v_m^{\gamma_m}$ in W is the number of walks of length α and final altitude β that have exactly γ_i occurrences of p_i for $i = 1, \dots, m$. (Note that occurrences of each pattern are taking self-overlaps into account: thus, for example, the path aaaa contains three occurrences of aa and two occurrences of aaa.)

▶ Remark 3 (The automaton paradigm). Given $\mathcal{S}$ and $\mathcal{P}$, walks with marked patterns can be encoded by a finite automaton $\mathcal{A}$: a walk w is in state Z_α if α is the longest overlap of w with some pattern(s) (if there are no such overlaps, then w is in the initial state Z_ϵ)[1]. This approach leads to the formula

$$W(t,u,v_1,\dots,v_m) = \frac{(1,0,\dots,0)\ \mathrm{adj}(I-tA)\ (1,\dots,1)^\top}{\det(I-tA)}, \tag{4}$$

where $A = A(u,v_1,\dots,v_m)$ is the transition matrix of the automaton $\mathcal{A}$. (NB: the first row/column of A correspond to the initial state Z_ϵ.) In Formula (4), the vector $(1,0,\dots,0)$ encodes the fact that the state Z_ϵ is the single initial state of $\mathcal{A}$, and the vector $(1,\dots,1)^\top$ encodes the fact that all states of $\mathcal{A}$ are final. (See the automaton in Example 9 for an illustration.)

Our first result is another more combinatorial formula for W, bypassing the computational cost inherent to the automaton paradigm approach. This formula can be established via the *cluster method*, as popularized by Goulden and Jackson [24]. It is an instance of what Flajolet called *symbolic inclusion-exclusion* and it was e.g. used in [1, 11, 32, 35, 39]. Below, we opt for another proof strategy which emphasizes the role of the mutual correlation polynomials.

▶ **Theorem 4.** *Let $\mathcal{S}$ be a set of steps, and $\mathcal{P} = \{p_1,\dots,p_m\}$ a set of (mutually not included) patterns. The* ***multivariate generating function of walks*** *(where t encodes the length, u the final altitude, and v_i occurrences of the pattern p_i) is given by*

$$W(t,u,v_1,\dots,v_m) = \frac{\Delta}{(1-tS(u))\Delta + \sum_{i=1}^{m} \Delta_i t^{\ell_i} u^{h_i}}, \tag{5}$$

where $\Delta = \Delta(t,u,v_1,\dots,v_m)$ is the determinant of the ***mutual correlation matrix***

$$\begin{pmatrix} v_1 + (1-v_1)C_{1,1} & (1-v_2)C_{2,1} & \cdots & (1-v_m)C_{m,1} \\ (1-v_1)C_{1,2} & v_2 + (1-v_2)C_{2,2} & \cdots & (1-v_m)C_{m,2} \\ \vdots & \vdots & \ddots & \vdots \\ (1-v_1)C_{1,m} & (1-v_2)C_{2,m} & \cdots & v_m + (1-v_m)C_{m,m} \end{pmatrix}, \tag{6}$$

and, for $i = 1,\dots,m$, $\Delta_i = \Delta_i(t,u,v_1,\dots,v_m)$ is the determinant of the matrix obtained from the mutual correlation matrix by replacing its ith row with $(1-v_1,\dots,1-v_m)$, and ℓ_i and h_i are the length and the final altitude of p_i.

Proof. It is convenient to introduce the generating function $W_i(t,u,v_1,\dots,v_m)$ of walks having p_i as a suffix. We first show that $W, W_1, \dots, W_m$ satisfy the equation

$$WtS = W - 1 + \sum_{j=1}^{m} (v_j^{-1} - 1) W_j. \tag{7}$$

To this end, we take a path $w \in \mathcal{W}$ and append a single letter $s \in \mathcal{S}$ at its end. If this produces no new occurrence of a pattern from $\mathcal{P}$, then $w.s$ is counted by $W - 1 - \sum_{j=1}^m W_j$. Otherwise, there is a new non-marked occurrence of a (uniquely determined) pattern $p_j \in \mathcal{P}$ at the end of $w.s$, and thus $w.s$ is counted by $v_j^{-1} W_j$. Now, as s can take all values in $\mathcal{S}$, this covers all the p_j's, and leads to the contribution $\sum_{j=1}^m v_j^{-1} W_j$.

[1] The notation Z, often used in statistical mechanics, is reminiscent of the word *Zustand*, which means *state* in German.

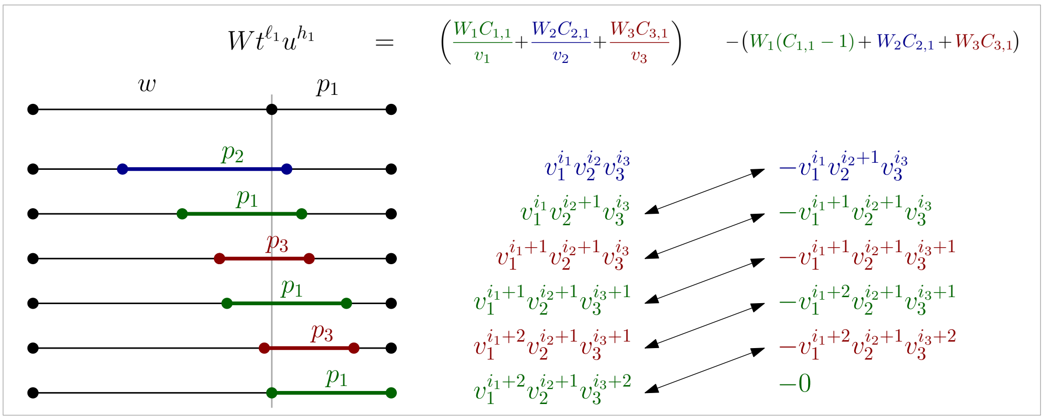
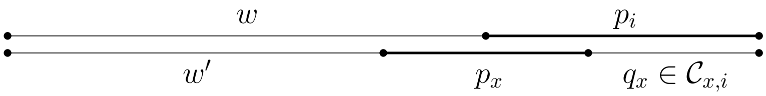


Figure 1 Illustration to the proof of Theorem 4. This schematic example (involving three patterns, p_1, p_2, and p_3) illustrates how the mutual correlation polynomials $C_{i,j}$ lead to the fact that the contributions of the decompositions $w'.p_x.q$ cancel out telescopically in the right-hand side of (8), and the full sum thus equals $v_1^{i_1}v_2^{i_2}v_3^{i_3}$, which is indeed the same as the contribution of the left-hand side of (8).

Next we show that, for each $i = 1, \ldots, m$, we have

$$Wt^{\ell_i}u^{h_i} = W_i + \sum_{j=1}^{m}(v_j^{-1} - 1)W_jC_{j,i}. \tag{8}$$

To prove this, we take a path $w \in \mathcal{W}$ and append the pattern p_i at its end, but do not mark any new occurrences of patterns from $\mathcal{P}$. For $j = 1, \ldots, m$, let γ_j be the number of occurrences of the pattern p_j in w. Then $w.p_i$ in the left-hand side of (8) contributes $v_1^{\gamma_1}v_2^{\gamma_2}\ldots v_m^{\gamma_m}$ to the generating function. Apart from p_i at the end, there are possibly some new occurrences of some patterns in $w.p_i$. Consider such a new occurrence of a pattern, say of p_x, in $w.p_i$. Then we have a decomposition $w.p_i = w'.p_x.q_x$, where $q_x \in \mathcal{C}_{x,i}$.



For $j = 1, \ldots, m$, let δ_j be the number of occurrences of the pattern p_j in $w'.p_x$. Then this decomposition contributes $v_1^{\delta_1}v_2^{\delta_2}\ldots v_m^{\delta_m}/v_x$ to $v_x^{-1}W_xC_{x,i}$, and $v_1^{\delta_1}v_2^{\delta_2}\ldots v_m^{\delta_m}$ to $W_xC_{x,i}$. Now consider the *next* new occurrence of a pattern, say of p_y, in $w.p_i$. The decomposition $w.p_i = w''.p_y.q_y$, where $q_y \in \mathcal{C}_{y,i}$, contributes $v_1^{\delta_1}v_2^{\delta_2}\ldots v_m^{\delta_m}$ to $v_y^{-1}W_yC_{y,i}$ and $v_1^{\delta_1}v_2^{\delta_2}\ldots v_m^{\delta_m}v_y$ to $W_yC_{y,i}$. Therefore, in the right-hand side of (8), the contributions of all the decompositions of $w.p_i$ will cancel out telescopically (we add W_i to cancel the contribution of $w.p_i$ itself), except the very first term whose contribution is $v_1^{\gamma_1}v_2^{\gamma_2}\ldots v_m^{\gamma_m}$. See Fig. 1 for illustration.

Finally, we regard (8) as an $m \times m$ linear system $C\mathbf{x} = \mathbf{d}$ with $\mathbf{x} = (W_1, \ldots, W_m)$ and $\mathbf{d} = (Wt^{\ell_1}u^{h_1}, \ldots, Wt^{\ell_m}u^{h_m})$. Let, further, $\mathbf{e} = (v_1^{-1}-1, \ldots, v_m^{-1}-1)$. We use the elementary fact that if $C\mathbf{x} = \mathbf{d}$ and $C^\top\mathbf{y} = \mathbf{e}$, then $\mathbf{x}\cdot\mathbf{e} = \mathbf{d}\cdot\mathbf{y}$, to find $\sum_{j=1}^{m}(v_j^{-1} - 1)W_j$. The solution $\mathbf{y}$ of $C^\top\mathbf{y} = \mathbf{e}$ can be written by Cramer's rule: we have $\mathbf{y} = \big(\det(C_1), \ldots, \det(C_m)\big)/\det(C)$, where C_i is the matrix obtained from C by replacing its ith *row* with $\mathbf{e}$. Therefore we have

$$\sum_{j=1}^{m}(v_j^{-1} - 1)W_j = \mathbf{x}\cdot\mathbf{e} = \mathbf{d}\cdot\mathbf{y} = \big(W/\det(C)\big)\sum_{i=1}^{m}t^{\ell_i}u^{h_i}\det(C_i). \tag{9}$$

We substitute this to (7), and solve for W. Finally, we multiply the numerator and the denominator by $v_1\ldots v_m$, and after some more rearrangement this yields the claimed formula (5). ◀

▶ Remark 5. Theorem 4 is a far-reaching generalization of several earlier results. For $v_1 = \ldots = v_m = 1$, we have $C = I$ and hence $\Delta = 1$, and $\Delta_i = 0$ for $1 = 1, \ldots, m$; thus $W(t, u, 1, \ldots, 1) = 1/(1-tS)$ as expected. For $v_1 = \ldots = v_m = 0$, we get the formula for walks that *avoid* $p_1, \ldots, p_m$, which was first obtained in [2]. For $m = 1$, we obtain [1, Thm. 7.1].

▶ Remark 6. Obtaining the generating function W by means of the finite automaton would generically require the inversion of an $L \times L$ matrix with symbolic coefficients, which is costly in time and in memory ($L := \sum_{i=1}^{m} \ell_i$ is the sum of the lengths of the marked patterns). It is nice that our formula based on the mutual correlation sets is algorithmically more efficient, and directly gives the generating function, avoiding those larger costs. However, comparing the two formulas for W leads to the following result (which will be used in the next section for our derivation of the closed-form formula for meanders).

▶ **Proposition 7.** *In the notation introduced above, we have*

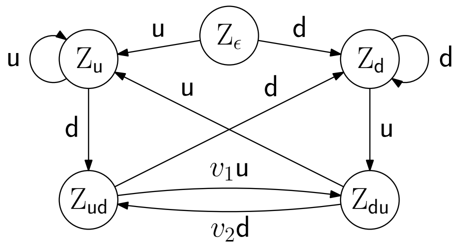
$$\Delta(t, u, v_1, \ldots, v_m) = (1, 0, \ldots, 0)\ \mathrm{adj}(I - tA)\ (1, \ldots, 1)^\top, \tag{10}$$

$$K(t, u, v_1, \ldots, v_m) := (1 - tS(u))\Delta + \sum_{i=1}^{m} \Delta_i t^{\ell_i} u^{h_i} = \det(I - tA). \tag{11}$$

Proof. Compare the formulas (4) and (5) for W, and notice that in both of them the denominator is polynomial in t with constant term 1. ◀

▶ **Definition 8.** *The expression K from* (11) *will be called the* ***kernel*** *of the walk.*

▶ **Example 9.** Consider Dyck walks (we denote the steps by $\mathsf{d} := -1$, $\mathsf{u} := 1$) with marked patterns $p_1 = \mathsf{udu}$ and $p_2 = \mathsf{dud}$. The following drawing shows the automaton for this model and its transition matrix A (the ordering of states is $Z_\epsilon, Z_\mathsf{u}, Z_\mathsf{ud}, Z_\mathsf{d}, Z_\mathsf{du}$).



$$A = \begin{pmatrix} 0 & u & 0 & u^{-1} & 0 \\ 0 & u & u^{-1} & 0 & 0 \\ 0 & 0 & 0 & u^{-1} & v_1 u \\ 0 & 0 & 0 & u^{-1} & u \\ 0 & u & v_2 u^{-1} & 0 & 0 \end{pmatrix}$$

We find $C_{1,1} = C_{2,2} = 1 + t^2, C_{1,2} = tu^{-1}, C_{2,1} = tu$; so, the mutual correlation matrix is

$$\begin{pmatrix} v_1 + (1 - v_1)(1 + t^2) & (1 - v_2)tu \\ (1 - v_1)tu^{-1} & v_2 + (1 - v_2)(1 + t^2) \end{pmatrix}.$$

By Theorem 4, we obtain the generating function for Dyck walks with marked p_1, p_2:

$$W(t, u, v_1, v_2) = \frac{1 + t^2(1 - v_1 v_2) + t^4(1 - v_1)(1 - v_2)}{1 - t(u^{-1} + u) + t^2(1 - v_1 v_2) - t^3\big(u^{-1}v_2(1 - v_1) + uv_1(1 - v_2)\big) - t^4(1 - v_1)(1 - v_2)}.$$

Setting v_1, v_2 to be 1 or 0, we allow or forbid the corresponding patterns. In this easy case, this recovers several known sequences, for example $W(t, u, 1, 1) = \dfrac{1}{1 - t(u^{-1} + u)}$ (as expected, since these are unrestricted walks); $W(t, 1, 0, 1) = W(t, 1, 1, 0) = \dfrac{1 + t^2}{1 - 2t + t^2 - t^3}$ (`A005251`)[2] ; $W(t, 1, 0, 0) = \dfrac{1 + t^2 + t^4}{1 - 2t + t^2 - t^4}$ (`A128588`, double Fibonacci numbers).

[2] This refers to the On-Line Encyclopedia of Integer Sequences (OEIS), available at https://oeis.org/.

▶ **Theorem 10.** *Let $\mathcal{S}$ be a set of steps, and $\mathcal{P} = \{p_1, \dots, p_m\}$ a set of (mutually not included) patterns. The* ***multivariate generating function of bridges*** *is given by*[3]

$$B(t, v_1, \dots, v_m) = \sum_{i=1}^{e} \frac{u_i'(t)}{u_i(t)} \frac{\Delta(t, u_i(t))}{K_t(t, u_i(t))}, \tag{12}$$

where $u_1(t), \dots, u_e(t)$ are the small roots of $K(t,u)$ (as defined in (11)*).*

Proof. To prove this formula, we extract $[u^0]$ from W, and obtain

$$B = [u^0](W) = \frac{1}{2\pi i}\int_{|u|=\varepsilon} \frac{W}{u} du = \sum_{i=1}^{e} \mathrm{Res}_{u=u_i} \frac{\Delta(t,u)}{uK(t,u)} = \sum_{i=1}^{e} \frac{\Delta(t,u_i)}{\frac{d}{du}(uK)(t,u_i)},$$

via Cauchy's integral formula and the residue theorem, where the poles inside $|u| = \varepsilon$ happen to be exactly the small roots u_i. Finally, the chain rule for total derivative yields Eq. (12). ◀

▶ **Example 11.** We return to the example considered above – Dyck walks with marked $p_1 = \mathsf{udu}$ and $p_2 = \mathsf{dud}$. By Theorem 10 we obtain the generating function for bridges:

$$B(t, v_1, v_2) = \sqrt{\frac{1 + \quad (1 - v_1 v_2)t^2 + (1 - v_1)(1 - v_2)t^4}{1 + (-3 - v_1 v_2)t^2 + (1 - v_1)(1 - v_2)t^4}},$$

which, in its turn, yields sequences that appeared in earlier work in different contexts such as patterns in binary strings, but also the Potts model from statistical mechanics: $B(t,1,1) = \frac{1}{\sqrt{1-4t^2}}$ (central binomial coefficients, as expected), $B(t,0,1) = B(t,1,0) = \sqrt{\frac{1+t^2}{1-3t^2}}$ (`A025565`, [3, 16, 30]), $B(t,0,0) = \sqrt{\frac{1+t^2+t^4}{1-3t^2+t^4}}$ (`A078678` [19, 34, 36]), etc.

3 Generating functions for meanders and excursions with marked patterns

While generating functions for walks can be found as a solution of a system of linear equations (which, in particular, implies that they are rational), the generating functions for meanders/excursions are typically algebraic (non-rational) and can be found by a suitable variation of the *kernel method*. One of them, the *vectorial kernel method*, was recently developed in [1] for dealing with enumerative problems encoded by a counter automaton. One of the cases in which this method leads to explicit formulas was that of meanders/excursions that avoid a single pattern p under the assumption that p itself is a meander. In this case, one has

$$M(t,u) = \frac{R(t,u)}{u^c K(t,u)} \prod_{i=1}^{c} (u - u_i(t)) \qquad \text{and} \qquad E(t) = -\frac{1}{t}\prod_{i=1}^{c}(-u_i(t)),$$

where c is the absolute value of the smallest number in $\mathcal{S}$, $R(t,u)$ is the autocorrelation polynomial, $K(t,u)$ is the kernel, and $u_1(t), \dots, u_c(t)$ are the small roots of $K(t,u)$. Our next theorem expands this result in two directions: first, it deals with several patterns, second, these patterns are marked and not just forbidden.

[3] Here and below we frequently remove the markers in the list of arguments of a function, writing $K(t,u)$, $\Delta(t,u)$, $u_i(t)$ for $K(t,u,v_1,\dots,v_m)$, $\Delta(t,u,v_1,\dots,v_m)$, $u_i(t,v_1,\dots,v_m)$, etc.

▶ **Theorem 12.** *Let $\mathcal{S}$ be a set of steps, and $\mathcal{P} = \{p_1, \ldots, p_m\}$ a set of (mutually not included) patterns, all of them being meanders themselves. Then the* ***multivariate generating function of meanders*** *is*

$$M(t, u, v_1, \ldots, v_m) = \frac{\Delta(t, u)}{u^c K(t, u)} \prod_{i=1}^{c} (u - u_i(t)), \tag{13}$$

where $K(t, u)$ is the kernel as in (11)*, $\Delta(t, u)$ is the determinant of the mutual correlation matrix* (6) *as in* (10)*, and $u_1(t), \ldots, u_c(t)$ are the small roots of $K(t, u)$.*
The ***multivariate generating function of excursions*** *is given by*

$$E(t, v_1, \ldots, v_m) = M(t, 0, v_1, \ldots, v_m) = -\frac{1}{t} \prod_{i=1}^{c} (-u_i(t)). \tag{14}$$

Proof. To prove (13), we apply the vectorial kernel method. According to its general scheme, we encode the meanders by the automaton, as explained before Theorem 4. We denote by M_i the generating function for meanders that terminate in state Z_i, and let $\mathbf{M} = (M_1, M_2, \ldots)$. Then we have the functional equation

$$\mathbf{M} = (1, 0, \ldots, 0) + t\mathbf{M}A - \{u^{<0}\}(t\mathbf{M}A), \tag{15}$$

where $\{u^{<0}\}(t\mathbf{M}A)$ consists of all terms of $t\mathbf{M}A$ that contain negative powers of u (in other words, $\{u^{<0}\}(t\mathbf{M}A)$ counts the paths $w.s$ such that w is a meander and $s \in \mathcal{S}$, and $w.s$ crosses the x-axis at its last step). Next we rewrite (15) as

$$\mathbf{M}(I - tA) = (1, 0, \ldots, 0) - \{u^{<0}\}(t\mathbf{M}A). \tag{16}$$

At this point we claim that in $\{u^{<0}\}(t\mathbf{M}A)$ only the first component is non-zero. This follows from the assumption that all our patterns are meanders. Therefore, if a walk $w.s$ as above has a *non-empty* overlap with $p \in \mathcal{P}$, it is impossible that its last step crosses the x-axis. This means that $w.s$ crosses the x-axis at its last step, then it is necessarily in state Z_ϵ. Therefore, negative powers of u can occur only in the first component of $t\mathbf{M}A$. Notice further that all the terms of $\{u^{<0}\}(t\mathbf{M}A)$ contain u to some powers between $-c$ and -1. Therefore we can multiply (16) by u^c and obtain

$$\mathbf{M}\, u^c\, (I - tA) = (F(t, u), 0, \ldots, 0), \tag{17}$$

where $F(t, u)$ is a monic polynomial in u of degree c.

Next we multiply (17) by $\operatorname{adj}(I - tA)(1, \ldots, 1)^\top$, and obtain, due to (10) and (11),

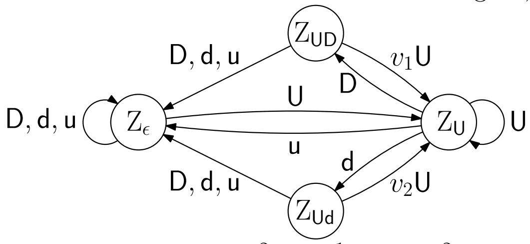
$$M(t, u)\, u^c\, K(t, u) = F(t, u)\Delta(t, u). \tag{18}$$

Here, it is legitimate to substitute, for u, any small root $u_i(t)$ of $K(t, u)$. Then the left-hand side of (18) vanishes. It is impossible that $\Delta(t, u_i(t)) = 0$ because $\Delta(t, u)$, as polynomial in t, has constant term 1 (this follows from the fact that $C_{i,i}(t, u)$ has constant term 1, and $C_{i,j}(t, u)$, $i \neq j$, has constant term 0). Therefore we have $F(t, u_i(t)) = 0$, that is, $u_i(t)$'s also are roots of $F(t, u)$.

Finally, $K(t, u)$ has precisely c small roots, $u_1(t), \ldots, u_c(t)$ (this can be proven in the same way as [1, Prop. 4.4]). Thus, $u_1(t), \ldots, u_c(t)$, are roots of $F(t, u)$, which is a monic polynomial of degree u. Therefore we know its decomposition, $F(t, u) = \prod_{i=1}^{c} (u - u_i(t))$. Now the formula (13) follows from (18).

To get (14), we substitute $u = 0$ and notice that the only term in the denominator that does not vanish is $-t\Delta$. ◀

▶ **Example 13.** Basketball walks are lattice paths with $\mathcal{S} = \{-2, -1, 1, 2\}$. We also denote their steps by $\mathsf{D} = -2$, $\mathsf{d} = -1$, $\mathsf{u} = 1$, $\mathsf{U} = 2$. In this example we find the generating functions for meanders and excursions with marked $p_1 = \mathsf{UDU}$ and $p_2 = \mathsf{UdU}$. The automaton and its transition matrix are shown in the next figure, the ordering of the states is $Z_\epsilon, Z_{\mathsf{U}}, Z_{\mathsf{UD}}, Z_{\mathsf{Ud}}$.



$$A = \begin{pmatrix} u^{-2}+u^{-1}+u & u^2 & 0 & 0 \\ u & u^2 & u^{-2} & u^{-1} \\ u^{-2}+u^{-1}+u & v_1u^2 & 0 & 0 \\ u^{-2}+u^{-1}+u & v_2u^2 & 0 & 0 \end{pmatrix}$$

We have $S(u) = u^{-2} + u^{-1} + u + u^2$ and $c = 2$. The mutual correlation polynomials are $C_{11} = 1 + t^2$, $C_{12} = t^2u$, $C_{21} = t^2$, $C_{22} = 1 + t^2u$. By Theorem 4, we obtain $\Delta = 1 + t^2 + t^2u$ and $K = -\big((t + t^3) + (t + 2t^3)u - (1 + t^2 - t^3)u^2 + (t - t^2 + t^3)u^3 + (t + t^3)u^4\big)/u^2$. Thus, u^2K is a polynomial of degree 4 with two small roots given by given by Puiseux series

$$u_{1,2}(t) = \pm t^{\frac{1}{2}} + \frac{1}{2}t \pm \frac{1}{8}t^{\frac{3}{2}} + \frac{1}{2}t^2 \pm \frac{159}{128}t^{\frac{5}{2}} + \frac{3}{2}t^3 \pm \frac{1761}{1024}t^{\frac{7}{2}} + \frac{7}{2}t^4 \pm \frac{213435 + 16384v_1}{32768}t^{\frac{9}{2}} + \frac{19 + 2v_1 + v_2}{2}t^5 \pm \ldots$$

By Theorem 12, we obtain generating functions for meanders/excursions with *marked* p_1, p_2:

$$M(t, u, v_1, v_2) = \frac{\Delta(t,u)}{u^2K(t,u)}(u - u_1(t))(u - u_2(t)) =$$
$$1 + (u + u^2)t + (2 + u + u^2 + 2u^3 + u^4)t^2 + (2 + 5u + (5 + v_1)u^2 + (2 + v_2)u^3 + 3u^4 + 3u^5 + u^6)t^3 + \ldots,$$
$$E(t, v_1, v_2) = \frac{u_1(t)u_2(t)}{-t} = 1 + 2t^2 + 2t^3 + (10 + v_1)t^4 + (21 + v_1 + 2v_2)t^5 + (79 + 9v_1 + 4v_2 + v_1^2)t^6 + \ldots$$

(For example, there is one excursion of size 5 that contains UDU, namely UDUdd, and two excursions that contain UdU, namely UdUdD, and UdUDd.)

To obtain the univariate generating functions for all meanders and that for excursions that *avoid* p_1, p_2, we substitute $v_1 = v_2 = 0$, and $u = 1$ resp. $u = 0$:

$$M(t) = 1 + 2t + 7t^2 + 21t^3 + 71t^4 + 245t^5 + 867t^6 + 3091t^7 + 11147t^8 + 40491t^9 + 148010t^{10} + \ldots,$$
$$E(t) = 1 + 2t^2 + 2t^3 + 10t^4 + 21t^5 + 79t^6 + 224t^7 + 771t^8 + 2462t^9 + 8409t^{10} + \ldots$$

▶ Remark 14. If some of the patterns are not meanders, then generically several components of $\{u^{<0}\}(t\mathbf{M}A)$ are non-zero. Therefore, in general one does not get simple equations as (17) and (18), and the formula (13) does not hold verbatim. However, it is then possible to use the approach introduced in [1, Thm. 3.2]; this gives that $M(t, u)$ has the form $\frac{G(t,u)}{u^cK(t,u)}\prod_{i=1}^{c}(u - u_i(t))$, where $G(t, u)$ is polynomial in u. There are other cases, not covered by Theorem 12, where it is possible to find formulas for $M(t, u)$ and $E(t, u)$. For example, if the only negative step in $\mathcal{S}$ is -1 (such paths are called *Łukasiewicz walks*), one can use the fact that a path can cross the x-axis only when a (-1)-step is appended to an excursion. Using further ideas developed (for avoidance) in [2], we can find, for example, generating functions for Dyck meanders/excursions with marked $p_1 = \mathsf{udu}, p_2 = \mathsf{dud}$:

$$M(t, u, v_1, v_2) = \left(1 - \frac{t^2(1 - v_1)(1 - v_2)}{2}\left(1 - \sqrt{1 - 4t^2/\Delta}\right)\right)\frac{\Delta}{uK}(u - u_1(t)),$$
$$E(t, v_1, v_2) = \frac{\Delta}{1 + t^2v_2(1 - v_1) + t^3(1 - v_1)(1 - v_2)u_1(t)}\frac{u_1(t)}{t} = \frac{\Delta}{2t^2}\left(1 - \sqrt{1 - \frac{4t^2}{\Delta}}\right),$$

where $\Delta = 1 + t^2(1 - v_1v_2) + t^4(1 - v_1)(1 - v_2)$ as found in Example 9 (note that another form of $E(t, v_1, v_2)$ is mentioned in `A145895`).

4 Multivariate Gaussian limit laws for pattern occurrences

4.1 Gaussian and multivariate Gaussian distribution

The Gaussian distribution is ubiquitous is mathematics, physics, biology, astronomy, finance, computer science, and even in human sciences, and, in fact, in any domain in which one could collect numerical data and do some statistics with them.

There are two frequent simple explanations of this universality.

- The first explanation is probabilistic: the central limit theorem of Laplace asserts that if one considers a sequence of independent and identically distributed random variables $(X_n)_{n\in\mathbb{N}}$ (with expected value μ and finite variance σ^2), then the sum $\sum_{k=1}^n X_k$ is converging towards the Gaussian distribution $\mathcal{N}(\mu,\sigma)$.
- The second explanation is analytic: if the corresponding probability generating function of $\operatorname{Prob}(X_n = k)$ behaves like a "quasi-power" (see [29]), then X_n has a Gaussian limit distribution.

Both approaches have their own interest, as both admit some flexibility in their condition of application. As masterfully presented by Flajolet and Sedgewick in [22], the second approach is typically split into two steps: first a combinatorial step consists in getting a closed-form expression (or a functional equation) for the generating function, and then a local analysis of this function near its dominant singularity is performed in order to get some universal behaviour (limit law, etc).

We apply a generalization of this analytico-combinatorial approach to the case of joint laws $\Pr(X_1 = k_1,\dots,X_m = k_m)$, including in cases where the random variables X_i are dependent. The dependence (the correlations) will be handled at the level of the generating function, on which some multivariate complex analysis is then performed in order to get the limit law. As a first step towards more examples in the realm of "multivariate analytic combinatorics" (as initiated in [12, 20, 28, 37]), we present here some results related to the multivariate Gaussian distribution.

For the tuple of random variables $\boldsymbol{X} = (X_1,\dots,X_m)$ of average $\boldsymbol{\mu} = (\mu_1,\dots,\mu_m)$ the associated covariance matrix $\boldsymbol{\Sigma}$ is defined by

$$\Sigma_{ij} := \mathbb{E}[(X_i-\mu_i)(X_j-\mu_j)] \qquad (\text{for } i,j = 1,\dots,m). \tag{19}$$

This matrix $\boldsymbol{\Sigma}$ is also sometimes called the variance-covariance matrix, as the diagonal terms are exactly the variance of each X_i. Note that $\boldsymbol{\Sigma}$ is a positive-definite matrix, therefore $\sqrt{\det\boldsymbol{\Sigma}}$ is well defined.

The multivariate Gaussian distribution (also called multivariate normal distribution, or m-dimensional Gaussian distribution, see e.g. [17]), denoted by $\mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})$, is a generalization of the classical (one-dimensional) normal distribution; its density is

$$\frac{1}{\sqrt{(2\pi)^m\det\boldsymbol{\Sigma}}}\exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right). \tag{20}$$

When all the bold quantities are scalars (i.e. when $m = 1$), it is coinciding with the classical expression for the density of the Gaussian distribution.

Let us now illustrate this multivariate approach on fundamental objects such as words and constrained lattice paths. We first present a nice unifying example, before switching to more general cases from the algebraic world.

4.2 A multi-multivariate generating function for all patterns at once

There is a vast amount of literature on Dyck, Motzkin, Schröder etc. lattice paths (or some related classes of RNA structures, ordered trees, permutations) in which some combination of patterns (valleys, peaks, etc.) are considered. Proofs of such results often rely on some ad hoc context-free grammar decompositions; see e.g. [10, 15, 18, 21, 31, 33]. The power of our approach is also in the fact that it enables us to obtain many such results *at once* by marking sufficiently many patterns and then setting them to be 0 or 1 in any desirable combinations.

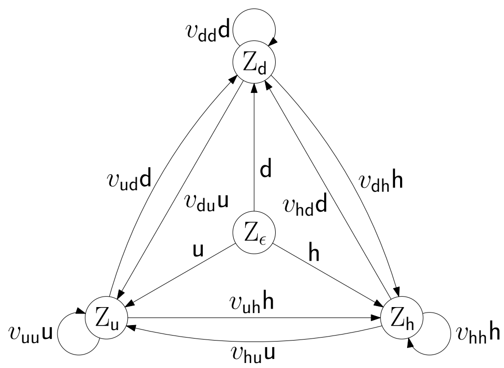
We illustrate this for the model of Motzkin walks ($\mathcal{S} = \{\mathsf{d} = -1, \mathsf{h} = 0, \mathsf{u} = 1\}$) in which we mark all possible patterns of length 2. To this aim, we introduce nine markers for all such patterns (v_{ud} for the pattern ud, etc.), and we obtain an even more explicit formula in cases not covered by the closed-form formula from Theorem 12. We give the general expression for excursions in the following theorem (the general expression for meanders is somewhat more lengthy, see also [2, Thm. 4]).

▶ **Theorem 15.** *The generating function $E(t, v_{\mathsf{uu}}, v_{\mathsf{uh}}, v_{\mathsf{ud}}, v_{\mathsf{hu}}, v_{\mathsf{hh}}, v_{\mathsf{hd}}, v_{\mathsf{du}}, v_{\mathsf{dh}}, v_{\mathsf{dd}})$ of Motzkin excursions, where each v_p counts the number of occurrences of the pattern p, is*

$$\frac{(v_{\mathsf{dd}}-1) - t((v_{\mathsf{dd}}-1)v_{\mathsf{hh}} - (v_{\mathsf{dh}}-1)v_{\mathsf{hd}} - v_{\mathsf{dd}} + v_{\mathsf{dh}}) + \big(1 + t(v_{\mathsf{dh}} - v_{\mathsf{hh}})\big)\frac{u\mathbf{v}_1}{t\mathbf{v}_4}\Big|_{u=u_1(t)}}{v_{\mathsf{dd}} + t(v_{\mathsf{dh}}v_{\mathsf{hd}} - v_{\mathsf{dd}}v_{\mathsf{hh}})}, \quad (21)$$

where $u_1(t)$ is the unique small solution of the kernel $K(t,u)$, and $\mathbf{v}_1$ and $\mathbf{v}_4$ are the 1st and the 4th components of $\mathbf{v} := \operatorname{adj}(I - tA)(1, \ldots, 1)^\top$.

Proof (Sketch). This model is encoded by the following automaton and its transition matrix:

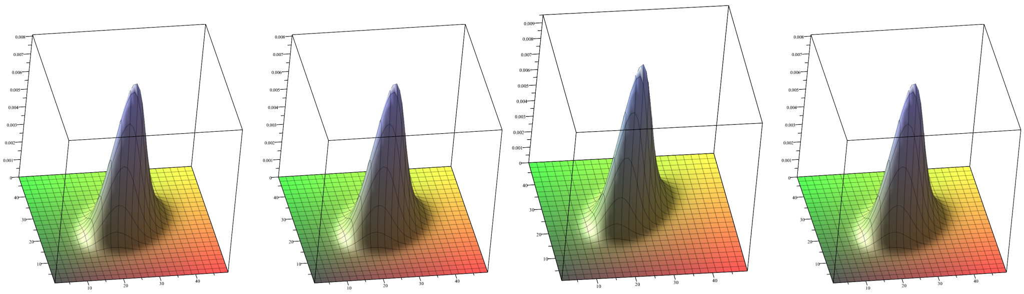


$$\begin{array}{cc} & \begin{array}{cccc} Z_\epsilon & Z_{\mathsf{u}} & Z_{\mathsf{h}} & Z_{\mathsf{d}} \end{array} \\ A = & \begin{pmatrix} 0 & u & 1 & u^{-1} \\ 0 & v_{\mathsf{uu}}u & v_{\mathsf{uh}} & v_{\mathsf{ud}}u^{-1} \\ 0 & v_{\mathsf{hu}}u & v_{\mathsf{hh}} & v_{\mathsf{hd}}u^{-1} \\ 0 & v_{\mathsf{du}}u & v_{\mathsf{dh}} & v_{\mathsf{dd}}u^{-1} \end{pmatrix} \end{array}$$

A Motzkin path can cross the x axis only by reading d (that is, entering the 4th state). Thus, only the fourth component of $t\mathbf{M}A$ has terms with negative powers of u. This leads to the equation $\mathbf{v}_1(t,u) - \mathbf{v}_4(t,u)N(t,u) = 0$ where $N(t,u)$ is the generating function for the terms with negative powers of u in the fourth component of $t\mathbf{M}A$. Note that by analyzing which patterns are read if $w.s$ crosses the x-axis, we can express N in terms of E.

Finally, as $uK(t,u)$ is a polynomial of degree 2 in u, it has one small root, $u_1(t)$ (we dropped the dependency on the other variables v_p's of the kernel (11)). Now, by the vectorial kernel method (see the proof of Theorem 12), this leads to the formula (21) for E. ◀

Setting the markers v_p to be 1 or 0 in all possible combinations leads to 512 specific models. An exhaustive analysis shows that they lead to 75 distinct sequences for excursions and 158 distinct sequences for meanders. In some cases we obtain new interpretations for existing OEIS entries, thus potentially leading to new bijections between different combinatorial structures.



walks $\mathbb{E}[X_i(n)] = \frac{n}{8} - \frac{1}{4}$ | bridges $\mathbb{E}[X_i(n)] \sim \frac{n}{8} - \frac{1}{8}$ | meanders $\mathbb{E}[X_i(n)] \sim \frac{n}{8} \pm \frac{\sqrt{2\pi n}}{16}$ | excursions $\mathbb{E}[X_i(n)] \sim \frac{n}{8} + \frac{1}{8}$

Figure 2 Distribution (X_1, X_2) of the pair of patterns (udu, dud) in a Dyck walks/bridges/meanders/excursions of length $n = 200$ (this corresponds to the model of Example 9). Already, for this small value of n, one sees that $\text{Prob}(X_1 = k_1, X_2 = k_2)$ is concentrated around the value $(\mathbb{E}[X_1], \mathbb{E}[X_2])$ with Gaussian fluctuations. (This example has by design a symmetric behaviour for X_1 and X_2 for walks, bridges, and excursions; this is not generically the case.)

Moreover, we checked that all these models satisfy the technical conditions (see [28, 37]) which ensure a *multivariate Gaussian distribution*. We now discuss more general models.

First, let us mention that the case of walks without positivity constraint or final altitude constraint is easier: indeed, their generating function W is rational, and one can then more directly apply results from [28, 36] to get the multivariate Gaussian distribution. Note that if one allows to mark a regular expression (and not just a finite set of words), then, already in the rational case, one can get "any" arbitrary (non-Gaussian) distribution (see [4] for a presentation of this huge diversity of the possible limit laws for pattern occurrences). It is more involved to analyse the algebraic generating function cases; one can however still prove that the multivariate Gaussian distribution also holds (see Figure 2 for an illustration):

▶ **Theorem 16.** *For any generic model of walks, let $X_i(n)$ be the random variable counting occurrences of the pattern p_i (for $i = 1, \ldots, m$) in a bridge/excursion/meander of length n. Then the joint law $(X_1(n), \ldots, X_m(n))$ convergences to a multivariate Gaussian distribution $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ as defined in Section 4.1.*

Proof (Sketch). Some technical conditions are required to avoid degenerated cases: for lattice paths, this corresponds to what is called *generic* model of walks in [1, Definition 6.1]; this definition includes conditions like having a unique dominant singularity, that the number of paths of length n is strictly increasing for large n, etc. Then, all the univariate asymptotics follow the universal asymptotics established in [1, 5, 6].

Now, the multivariate asymptotics follow the algebraic schemes investigated in [23, 26], and thus lead to the multivariate Gaussian distribution. It is also possible to use a multivariate Spitzer/Sparre Andersen formula (see [8, Theorem 8]), rephrased as

$$W^+(t, u, v_1, \ldots, v_m) := \{u^{\geqslant 0}\} W(t, u, v_1, \ldots, v_m) = [s^0] W(t, su, v_1, \ldots, v_m) 1/(1 - 1/s),$$
$$M(t, u, v_1, \ldots, v_m) \sim \exp \int_0^t \frac{W^+(z, u, v_1, \ldots, v_m) - 1}{z} dz. \tag{22}$$

In fact, Formula (22) is an equality when $v_i = 1$ (for $i = 1, \ldots, m$), while, if one keeps track of the v_i's, the counting of occurrences of p_i (in a meander of length n) could differ by a few $O(1)$ occurrences between both sides of Formula (22): indeed, the proof uses a concatenation of some final and initial parts of the path, and this can create/delete a few occurrences of p_i's.

The advantage of using the multivariate Spitzer formula is that this relates the meanders to a diagonal involving the rational generating function of walks, on which one can apply the results of [36]; the drawback is that one loses asymptotics below the $O(1)$ precision.

Let us now state how to derive the parameters of the multidimensional Gaussian limit law $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Let $F(t, u, v_1, \ldots, v_m)$ be the corresponding generating function (where t encodes the length, u the final altitude, and each v_i encodes occurrences of the pattern p_i). The average of the marginals behaves linearly, as expected by the Borges theorem (see [1,22]):

$$\mathbb{E}[X_i(n)] = \frac{[t^n]\partial_{v_i}(F)(t, 1, \ldots, 1)}{[t^n]F(t, 1, \ldots, 1)} = \mu_i n(1 + o(1)). \tag{23}$$

Note that, in (23), there would be no difficulty in pushing the asymptotics further than $o(1)$. One sets $\boldsymbol{\mu} := (\mu_1, \ldots, \mu_m)$. Now, the entries of the covariance matrix $\boldsymbol{\Sigma}$ are obtained by

$$\begin{aligned} \boldsymbol{\Sigma}_{ij} &= \lim_{n\to\infty} \frac{1}{n^2} \mathbb{E}\left[(X_i(n) - \mathbb{E}[X_i(n)])\,(X_j(n) - \mathbb{E}[X_j(n)])\right] \\ &= \lim_{n\to\infty} \frac{1}{n^2} \frac{[t^n]\partial_{v_i}\partial_{v_j}(F)(t, 1, \ldots, 1)}{[t^n]F(t, 1, \ldots, 1)} - \mu_i\mu_j. \end{aligned} \tag{24}$$

One has $\boldsymbol{\Sigma}_{ij} > 0$ as a consequence of the universal positivity of the variability condition [8, Lemma 22]) and $\det \boldsymbol{\Sigma} \neq 0$ when the patterns p_i's are not all equal.

Thus, when one considers the asymptotic regime of $[z^n v_1^{\mu_1 n} \ldots v_m^{\mu_m n}]F(z, v_1, \ldots, v_m)$, where the exponents of the v_i's can be rounded to the nearest integer whenever needed, one gets an expansion which fits the framework of the multivariate version of the quasi-power theorem (see [28,29,37]), leading to the multidimensional Gaussian limit law $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. ◀

▶ Remark. Generic walks are aperiodic; a multivariate Gaussian distribution is also holding for periodic walks, but additional care is required. (Recall that a walk is periodic if the gcd of the differences between the steps of $\mathcal{S}$ is not 1, and then the paths live in a periodic sub-lattice of $\mathbb{Z}^2$, and then the generating function has conjugate dominant singularities.) These periodic cases can in fact be handled by combining the approaches of [5] and [9].

5 Conclusion and further works

To summarize, in this article we introduced/presented

- the mutual correlation matrix, an extension of the notion of autocorrelation polynomial, which has its own interest and which offers several algorithmic advantages,
- closed-forms for all the main generating functions of constrained lattice paths (walks and bridges in Section 2, meanders and excursions in Section 3), generalizing the previous works [1,2,6] and leading to multidimensional Gaussian limit laws.

This will allow us to tackle further questions, like

- faster uniform random generation of constrained paths of length n, extending the multivariate tuning of the Boltzmann method done in [14] to cases where the grammar is not strongly connected (such cases are generic for lattice paths with forbidden patterns),
- links with trace monoids and partial commutations in words [13],
- to extend the analysis of fundamental non-Gaussian parameters under some pattern constraints (like the area below the path [7] for walks with forbidden patterns, thus interfering with the natural drift of the walk), possibly combined with further constraints (like to be below a line of rational slope, extending [9]).

This work is also a first step towards more general schemes of multidimensional limit laws in analytic combinatorics, for the important class of algebraic functions related to lattice path statistics.

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Latticepathology and Symmetric Functions (Extended Abstract)

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Abstract

In this article, we revisit and extend a list of formulas based on lattice path surgery: cut-and-paste methods, factorizations, the kernel method, etc. For this purpose, we focus on the natural model of directed lattice paths (also called generalized Dyck paths). We introduce the notion of prime walks, which appear to be the key structure to get natural decompositions of excursions, meanders, bridges, directly leading to the associated context-free grammars. This allows us to give bijective proofs of bivariate versions of Spitzer/Sparre Andersen/Wiener–Hopf formulas, thus capturing joint distributions. We also show that each of the fundamental families of symmetric polynomials corresponds to a lattice path generating function, and that these symmetric polynomials are accordingly needed to express the asymptotic enumeration of these paths and some parameters of limit laws. En passant, we give two other small results which have their own interest for folklore conjectures of lattice paths (non-analyticity of the small roots in the kernel method, and universal positivity of the variability condition occurring in many Gaussian limit law schemes).

2012 ACM Subject Classification Mathematics of computing → Generating functions; Mathematics of computing → Distribution functions; Theory of computation → Random walks and Markov chains; Theory of computation → Grammars and context-free languages

Keywords and phrases Lattice path, generating function, symmetric function, algebraic function, kernel method, context-free grammar, Sparre Andersen formula, Spitzer's identity, Wiener–Hopf factorization

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.2

Funding This work was initiated during the sojourn of Marie-Louise Lackner and Michael Wallner at the University of Paris Nord, via a Franco-Austrian "Amadeus" project and via a MathStic funding. The subsequent part of this collaboration was funded by the Erwin Schrödinger Fellowship of the Austrian Science Fund (FWF): J 4162-N35.

Acknowledgements We thank our referees for their careful reading. In this period of worldwide lockdown due to the COVID19 pandemic, let us also thank Klaus Hulek, Barbara Strazzabosco, and the staff from zbMATH who implemented some technical solution so that we can have home access to this wonderful database.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 2; pp. 2:1–2:16
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

1 Introduction and definitions

The recursive nature of lattice paths makes them amenable to context-free grammar techniques; their geometric nature makes them amenable to cut-and-paste bijections; their step-by-step nature makes them amenable to functional equations solvable by the kernel method (see e.g. [3–5, 8–11, 16, 30, 32, 35] for many applications of these ideas). We present in a unified way some consequences of these observations in Section 2 on context-free grammars (where we introduce the fruitful notion of prime walks) and in Section 3 on Spitzer and Wiener–Hopf identities. Additionally, we give new connections with symmetric functions in Section 4, see Table 2. All of this allows us to greatly extend the enumerative formulas and asymptotics given in [4], and gives us access to some limit laws, as shown in Section 5.

▶ **Definition 1** (Jumps and lattice paths). *A step set $\mathcal{S}$ is a finite subset of $\mathbb{Z}$. The elements of $\mathcal{S}$ are called steps or jumps. An n-step lattice path or walk ω is a sequence $(j_1, \dots, j_n) \in \mathcal{S}^n$. The length $|\omega|$ of this lattice path is its number n of jumps.*

Such sequences are one-dimensional objects. Geometrically, they can be interpreted as two-dimensional objects which justifies the name *lattice path*. Indeed, $(j_1, \dots, j_n)$ may be seen as a sequence of points $(\omega_0, \omega_1, \dots, \omega_n)$, where ω_0 is the starting point and $\omega_i - \omega_{i-1} = (1, j_i)$ for $i = 1, \dots, n$. Except when mentioned differently, the starting point ω_0 of these lattice paths is $(0, 0)$.

Let $\sigma_k := \sum_{i=1}^{k} j_i$ be the partial sum of the first k steps of the walk ω. We define the *height* or *maximum of* ω as $\max_k \sigma_k$, and the *final altitude of* ω as σ_n. For example, the first walk in Table 1 has height 3 and final altitude 1. Table 1 and Figure 1 are also illustrating the four following classical types of paths:

▶ **Definition 2** (Excursions, arches, meanders, bridges).

- *Excursions are paths never going below the x-axis and ending on the x-axis;*
- *Arches are excursions that only touch the x-axis twice: at the beginning and at the end;*
- *Meanders are prefixes of excursions, i.e., paths never going below the x-axis;*
- *Bridges are paths ending on the x-axis (allowed to cross the x-axis any number of times).*

Let $c := -\min \mathcal{S}$ be the maximal negative step, and let $d := \max \mathcal{S}$ be the maximal positive step. To avoid trivial cases we assume $\min \mathcal{S} < 0 < \max \mathcal{S}$. Furthermore we associate to each step $i \in \mathcal{S}$ a weight s_i. These weights s_i are typically real numbers, like probabilities or non-negative integers encoding the multiplicity of each jump. The weight of a lattice path is the product of the weights of its steps. Then we associate to this set of steps the following *step polynomial*:

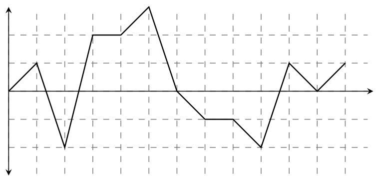
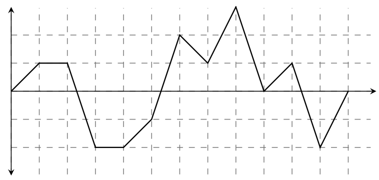
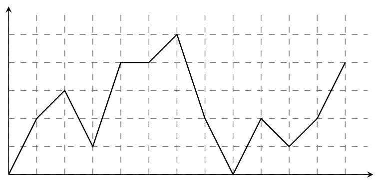
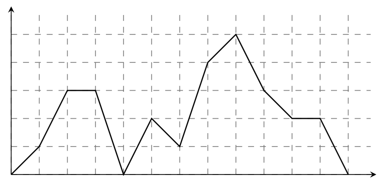
$$S(u) = \sum_{i=-c}^{d} s_i u^i.$$

The generating functions of directed lattice paths can be expressed in terms of the roots of the *kernel equation*

$$1 - zS(u) = 0. \tag{1}$$

More precisely, this equation has $c + d$ solutions in u. The *small roots* $u_i(z)$, for $i = 1, \dots, c$, are the c solutions with the property $u_i(z) \sim 0$ for $z \sim 0$. The remaining d solutions are called *large roots* as they satisfy $|v_i(z)| \sim +\infty$ for $z \sim 0$. The generating functions of the four classical types of lattice paths introduced above are shown in Table 1.

Table 1 The four types of paths: walks, bridges, meanders and excursions, and the corresponding generating functions for directed lattice paths. The functions $u_i(z)$ for $i = 1, \dots, c$ are the roots of the kernel equation $1 - zS(u) = 0$ such that $\lim_{z=0} u_i(z) = 0$.

	ending anywhere	ending at 0
unconstrained (on $\mathbb{Z}$)	 walk/path ($\mathcal{W}$) $W(z) = \frac{1}{1-zS(1)}$	 bridge ($\mathcal{B}$) $B(z) = z \sum_{i=1}^{c} \frac{u_i'(z)}{u_i(z)}$
constrained (on $\mathbb{Z}$)	 meander ($\mathcal{M}$) $M(z) = \frac{1}{1-zS(1)} \prod_{i=1}^{c} (1 - u_i(z))$	 excursion ($\mathcal{E}$) $E(z) = \frac{(-1)^{c-1}}{s_{-c}z} \prod_{i=1}^{c} u_i(z)$

These results follow from the expression for the bivariate generating function $M(z, u)$ of meanders. Indeed, let $m_{n,k}$ be the number of meanders of length n going from altitude 0 to altitude k, then we have

$$M(z,u) = \sum_k M_k(z)u^k = \sum_{n,k \geqslant 0} m_{n,k} z^n u^k = \frac{\prod_{i=1}^{c}(u - u_i(z))}{u^c(1 - zS(u))}. \tag{2}$$

This last formula is obtained by the kernel method: this method starts with the functional equation which mimics the recursive definition of meanders, namely $M(z, u) = 1 + zS(u)M(z, u) - \{u^{<0}\}zS(u)M(z, u)$ (where $\{u^{<0}\}$ extracts the monomials of negative degree in u, as one does not want to allow a jump going below the x-axis). Note that $\{u^{<0}\}S(u)M(z, u)$ is a linear combination (with coefficients in u and z) of c unknowns, namely $M_0(z), \dots, M_{c-1}(z)$. Then, substituting $u = u_i(z)$ (each of the c small roots of (1)) into this system leads to the closed form (2). This also directly gives the generating function of excursions $E(z) := M(z, 0)$ and meanders $M(z) := M(z, 1)$. The generating function for bridges follows from the link given in Theorem 8 hereafter. See [4, 10] for more details.

It should be stressed that the closed forms of Table 1 grant easy access to the asymptotics of all these classes of paths after the localization of the dominant singularities:

▶ **Theorem 3** (Radius of convergence of excursions, bridges, and meanders [4]). *The radius of convergence of excursions $E(z) := M(z, 0)$ and of bridges $B(z)$ is given by $\rho = 1/S(\tau)$, where τ is the smallest positive real number such that $S'(\tau) = 0$. For meanders $M(z) := M(z, 1)$, the radius depends on the drift $\delta := S'(1)$: It is ρ if $\delta < 0$ and it is $1/S(1)$ if $\delta \geqslant 0$.*

We shall make use of all these facts in Section 5 on asympotitcs and limit laws, but, before to do so, we now present several combinatorial decompositions which will be the key to get these new asymptotic results.

2 Prime walks and context-free grammars

Context-free grammars are a powerful tool to tackle problems related to directed lattice paths (we refer to [27] for a detailed presentation of grammar techniques). In this section, we introduce some key families of lattice paths (generalized arches, prime walks), which will also be used in the next section. Illustrating the philosophy of "latticepathology", these new families allow short concise visual proofs based on lattice path surgery: we give grammars generating the most fundamental classes of lattice paths (excursions, bridges, meanders); this generalizes and unifies results from [11, 16, 32, 35].

All our grammars are non-ambiguous: there is only one way to generate each lattice path. They require the introduction of two classes of paths: *generalized arches* and *prime walks.*

▶ **Definition 4** (Generalized arches)**.** *An arch from i to j is a walk starting at altitude i ending at altitude j and staying always strictly above altitude* $\max(i, j)$ *except for its first and final position; see Figure 1.*

An important consequence of this definition is that generalized arches cannot have an excursion as left or right factor. Note that an arch from i to j can be considered as an arch from 0 to $j - i$. This justifies that we now focus on arches starting at 0. Let $\mathcal{A}_k$ be the class of arches from 0 to k; see Figure 1. Following the tradition of several authors, we refer to *arches* (omitting the start and end point) as arches from 0 to 0, see e.g. [4]. Thus, an excursion is clearly a sequence of arches.

▶ **Definition 5** (Prime walks)**.** *Given a set of steps $\mathcal{S}$, with $d = \max \mathcal{S}$, the set $\mathcal{P}$ of prime walks is defined as the following sets of arches*

$$\mathcal{P} = \bigcup_{k=0}^{d} \mathcal{A}_k .$$

These prime walks are the key to get short proofs for the decomposition of several constrained classes of paths (Section 3) and for meanders (Theorem 6). Note that these decompositions hold for any set of jumps: it is straightforward to extend them to multiplicities (jumps with different colours) or even to an infinite set of jumps.

▶ **Theorem 6** (The universal context-free grammar for directed lattice paths)**.** *Meanders and excursions are generated by the following grammar:*

$$\begin{array}{lcll} \mathcal{M} & \to & \varepsilon + \mathcal{P}\,\mathcal{M} & \textit{(meanders)}, \\ \mathcal{E} & \to & \varepsilon + \mathcal{A}_0 \mathcal{E} & \textit{(excursions)}, \end{array}$$

which can be rephrased as "meanders are sequences of prime walks": $\mathcal{M} = \mathrm{Seq}\left(\sum_{k=0}^{d} \mathcal{A}_k\right)$ *and "excursions are sequences of arches":* $\mathcal{E} = \mathrm{Seq}(\mathcal{A}_0)$*, where the arches $\mathcal{A}_k$ from 0 to k are generated by*

$$\begin{array}{lcll} \mathcal{A}_k & \to & k + \displaystyle\sum_{j=k+1}^{d} \mathcal{A}_j \, \mathcal{E} \, \mathcal{A}_{k-j} & (\textit{arches for } k \geqslant 0), \\ \mathcal{A}_k & \to & k + \displaystyle\sum_{j=-c}^{k-1} \mathcal{A}_{k-j} \, \mathcal{E} \, \mathcal{A}_j & (\textit{arches for } k < 0), \end{array}$$

with the convention that, in these two rules, the part $\mathcal{A}_k \to k$ is omitted whenever $k \notin \mathcal{S}$.

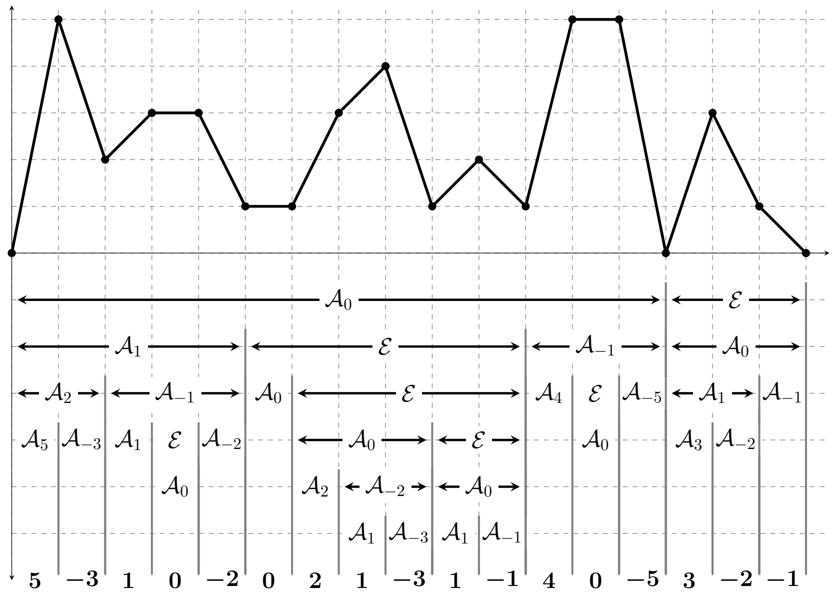


Figure 1 Example of our non-ambiguous decomposition of an excursion into generalized arches. Similar decompositions hold for the factorization of meanders into prime walks.

Proof. Let us start with arches $\mathcal{A}_k$ from 0 to $k \geqslant 0$. (The results for $\mathcal{A}_{-k}$ follow analogously.) For such arches of length > 1, we cut them at the first and the last time their minimal altitude (not taking end points into account) is attained. The first factor goes from 0 to j and stays in-between always strictly above j, and therefore is given by $\mathcal{A}_j$. The second factor is a (possibly empty) excursion. The last factor is an arch from j to k given by $\mathcal{A}_{k-j}$. This gives $\mathcal{A}_k = \mathcal{A}_j\mathcal{E}\mathcal{A}_{k-j}$. From this, it is immediate to get the grammar for excursions, as they are a sequence of arches $\mathcal{A}_0$; thus $\mathcal{E} = \varepsilon + \mathcal{A}_0\mathcal{E}$.

Now take any meander and cut it at the last time it touches altitude 0. The first part is a (possibly empty) sequence of arches. We cut the second part at the first point where its minimal altitude > 0 is attained. The remaining part is again a meander. This gives the factorization $\mathcal{M} = \mathcal{E} + \sum_{k=1}^{d} \mathcal{E}\,\mathcal{A}_k\,\mathcal{M}$, which is in turn equivalent to $\mathcal{M} = \operatorname{seq}(\mathcal{P})$.

All these decompositions are clearly 1-to-1 correspondences, as exemplified in Figure 1. ◀

We end this section with the grammar of bridges. It uses another class of walks: the negative arches from 0 to k, denoted by $\bar{\mathcal{A}}_k$. These stay always strictly below $\min(0,k)$. Their grammar is just the mirror of the one for $\mathcal{A}_k$ given in Theorem 6.

▶ **Theorem 7.** *Bridges $\mathcal{B} = \mathcal{B}_0$ are generated by the following grammar:*

$$\mathcal{B}_0 \quad \rightarrow \quad \varepsilon + \sum_{k\in\mathcal{S}} k\mathcal{B}_{-k},$$

where $\mathcal{B}_k$ stands for the "bridges ending at k", i.e. walks on $\mathbb{Z}$ from 0 to k, given by

$$\mathcal{B}_k \quad \rightarrow \quad \sum_{j=-c}^{0} \mathcal{A}_j\,\mathcal{B}_{k-j} \qquad \text{(if } k > 0\text{)},$$

$$\mathcal{B}_k \quad \rightarrow \quad \sum_{j=0}^{d} \bar{\mathcal{A}}_j\,\mathcal{B}_{k-j} \qquad \text{(if } k < 0\text{)}.$$

In the next section we present some applications of our decompositions (obtained above in the framework of the non-commutative world of words) to famous identities from probability theory (stated below in the framework of the commutative world of generating functions).

3 Latticepathology and surgery of paths

The decompositions of lattice paths mentioned in the previous section find application in the bivariate versions of the Spitzer/Sparre Andersen[1]/Wiener–Hopf formulas [2, 25, 26, 34, 37]. It gives for free elegant short proofs for these fundamental results which were definitively missing in [4], neatly illustrating the latticepathology philosophy!

▶ **Theorem 8** (Bivariate version of Spitzer/Sparre Andersen's identities). *The generating function $W^+(z,u) = \sum_n w_n^+(u)z^n$ of walks on $\mathbb{Z}$ ending at an altitude $\geqslant 0$ and the generating function $M(z,u) = \sum_n m_n(u)z^n$ of meanders (where u encodes the final altitude and z encodes the length of the lattice path) are related by the formulas*

$$W^+(z,u) = 1 + z\frac{M'(z,u)}{M(z,u)} \qquad \text{or, equivalently,} \tag{3a}$$

$$M(z,u) = \exp\left(\int_0^z \frac{W^+(t,u)-1}{t}\,dt\right) = \exp\left(\sum_{n\geqslant 1} \frac{w_n^+(u)}{n} t^n\right). \tag{3b}$$

Proof (Sketch). We give a bijective proof. It consists in factorizing any non-empty walk ω ending at an altitude $\geqslant 0$ into 3 factors: $\omega = \phi_1.m.\phi_2$ where m is the longest meander starting at the first minimum of the walk and such that $\phi_2.\phi_1$ is a prime walk (pointed, in order to remember where to split it); see Figure 2. The fact that this factorization exists and is unique follows from the positivity of ω and from the grammar for meanders from Theorem 6. This decomposition directly keeps track of the last altitude of each of its factors:

$$W^+(z,u) - 1 = M(z,u)z\frac{\partial}{\partial z}\left(1 - \frac{1}{M(z,u)}\right). \qquad ◀$$

▶ Remark 9 (Spitzer/Sparre Andersen's identities for excursions and bridges). Extracting the constant coefficient with respect to u in the above identities leads to the following links between bridges and excursions (these specific identities were also proven in [4]).

$$B(z) = 1 + E(z)z\frac{\partial}{\partial z}\left(1 - \frac{1}{E(z)}\right) = 1 + z\frac{E'(z)}{E(z)} \qquad \text{or, equivalently,} \tag{4a}$$

$$E(z) = \exp\left(\int_0^z \frac{B(t)-1}{t}\,dt\right) = \exp\left(\sum_{n\geqslant 1} \frac{b_n}{n} t^n\right). \tag{4b}$$

Nota bene: Spitzer's formula is often given as a variant of Formula (3b), stated in terms of characteristic functions instead of generating functions, and also keeping track of the height of the path (see e.g. [37,39,42]). More generally, in Brownian motion theory, path decompositions are also useful for Vervaat transformations, quantile transforms [13, 33, 40], Ray–Knight theorems for local times and Lamperti, Jeulin, Bougerol, Donati-Martin identities [1,7,15,28].

We now illustrate such approaches with one more important surgery of lattice paths. (This requires the natural classes of positive and negative meanders, see Definition 12 hereafter.)

[1] Funnily, in the literature, this identity of Erik Albrecht Sparre Andersen (Andersen is the family name) is often called the "Sparre Andersen identity", probably as he was often signing E. Sparre Andersen.

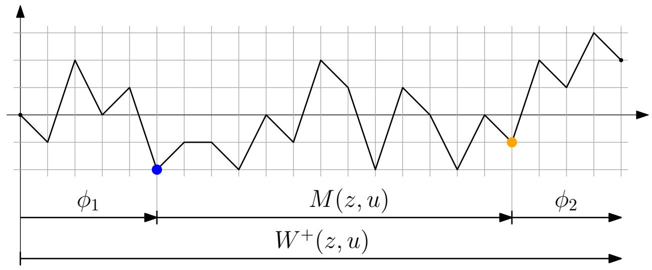


Figure 2 The bijection at the heart of Spitzer/Sparre Andersen identity decomposes a walk $\omega \in \mathcal{W}^+$ into $\omega = \phi_1.m.\phi_2$, where the meander $m \in \mathcal{M}$ starts at the first minimum of ω and ends at the rightmost point such that $\phi_2.\phi_1$ ends at altitude $\geqslant 0$ (and $\phi_2.\phi_1$ is thus a prime walk).

▶ **Theorem 10** (Bivariate version of Wiener–Hopf formula). *The bivariate generating functions $W_{+h}(z,u)$ and $W_{-h}(z,u)$ of walks on $\mathbb{Z}$ with u marking the positive and negative height (not the altitude!) are related to the bivariate generating functions $M^+(z,u)$ of positive meanders and $M^-(z,u)$ of negative meanders (with u marking the final altitude, see Figure 3):*

$$W_{+h}(z,u) = M^-(z)E(z)M^+(z,u) = -\frac{1}{s_d z}\left(\prod_{j=1}^{c}\frac{1}{1-u_j(z)}\right)\left(\prod_{\ell=1}^{d}\frac{1}{u-v_\ell(z)}\right),$$

$$W_{-h}(z,u) = M^-(z,u)E(z)M^+(z) = -\frac{1}{s_d z}\left(\prod_{j=1}^{c}\frac{1}{1-u_j(z)/u}\right)\left(\prod_{\ell=1}^{d}\frac{1}{1-v_\ell(z)}\right).$$

This Wiener–Hopf factorization $W = M^-EM^+$ thus gives

$$M^-(z) = \frac{W(z)}{M(z)} = \prod_{j=1}^{c}\frac{1}{1-u_j(z)} \qquad \text{and} \qquad M^+(z) = \frac{M(z)}{E(z)} = \prod_{\ell=1}^{d}\frac{1}{1-1/v_\ell(z)}.$$

Proof (Sketch). The proof follows from the decomposition illustrated in Figure 3. Cutting at the first and last maxima of the walk gives the factorization $\mathcal{W} = \mathcal{M}^+\mathcal{E}\mathcal{M}^-$, where the positive meander and the excursion are obtained after a 180^o rotation, and it is thus clear that the final altitude of this positive meander is the height of the initial walk. Similarly, cutting the walk at its first and last minima gives the factorization $\mathcal{W} = \mathcal{M}^-\mathcal{E}\mathcal{M}^+$. ◀

4 Lattice paths and symmetric functions

Building on the quantities introduced in the previous sections, we now show that three fundamental classes of symmetric polynomials evaluated at the small roots of the kernel have a natural combinatorial interpretation in terms of directed lattice paths. *En passant*, this also gives the generating function of generalized arches. For our main results see Table 2. We first recall the definitions of these symmetric polynomials (see e.g. [38] for more on these objects).

▶ **Definition 11.** *The complete homogeneous symmetric polynomials h_k of degree k in the d variables $x_1, \dots, x_d$ are defined as*

$$h_k(x_1,\dots,x_d) = \sum_{1\leqslant i_1\leqslant\cdots\leqslant i_k\leqslant d} x_{i_1}\cdots x_{i_k}, \qquad \text{thus} \sum_{k\geqslant 0} h_k(x_1,\dots,x_d)u^k = \prod_{i=1}^{d}\frac{1}{1-ux_i}. \tag{5}$$

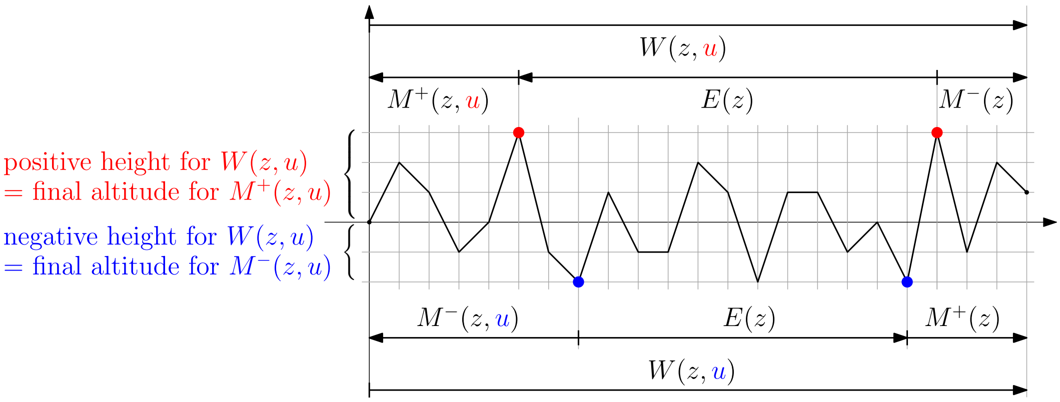


Figure 3 The Wiener–Hopf decomposition of a walk: $\mathcal{W} = \mathcal{M}^-\mathcal{E}\mathcal{M}^+$, a product of a negative meander, an excursion, and a positive meander. See e.g. [25] for the importance of this factorization for lattice path enumeration. It offers a link between two important parameters (height and final altitude): the proof uses a 180^o rotation of some of the factors (the ones indicated by a right to left arrow in the picture). The above picture crystallizes the key idea behind the theorems given by Feller in his nice introduction to the Wiener–Hopf factorization [19, Chapter XVIII.3 and XVIII.4]. It also explains why this decomposition holds for Lévy processes, which can be seen as the continuous time and space version of lattice paths, see [31].

The elementary homogeneous symmetric polynomials e_k of degree k in the d variables $x_1, \ldots, x_d$ are defined as

$$e_k(x_1,\ldots,x_d) = \sum_{1\leqslant i_1<\cdots<i_k\leqslant d} x_{i_1}\cdots x_{i_k}, \qquad \text{thus } \sum_{k=0}^{c} e_k(x_1,\ldots,x_d)u^k = \prod_{i=1}^{d}(1+ux_i). \tag{6}$$

The power sum homogeneous symmetric polynomials p_k of degree k in the d variables $x_1, \ldots, x_d$ are defined as

$$p_k(x_1,\ldots,x_d) = \sum_{i=1}^{d} x_i^k, \qquad \text{thus } \sum_{k\geqslant 0} p_k(x_1,\ldots,x_d)u^k = \sum_{i=1}^{d}\frac{1}{1-ux_i}. \tag{7}$$

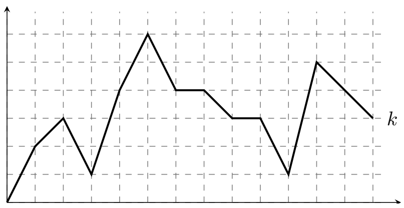
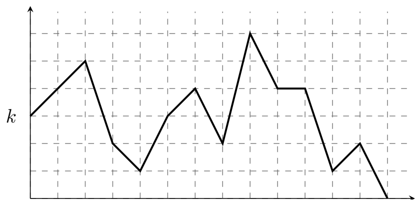
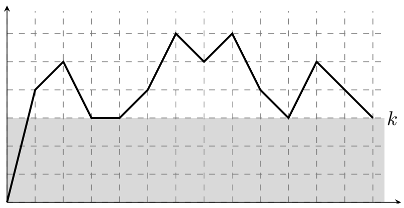
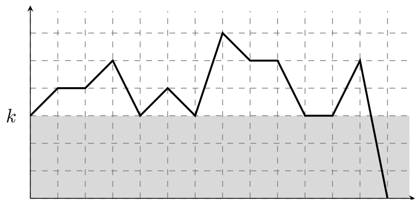
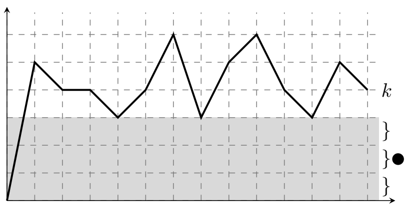
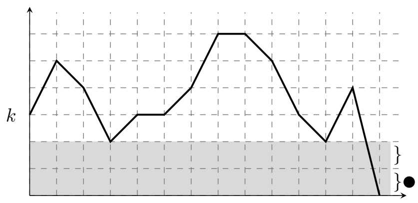
Many variants of directed lattice paths satisfy functional equations which are solvable by the kernel method and lead to formulas involving a quotient of Vandermonde-like determinants, see e.g. [4]. It is thus natural that Schur polynomials intervene, they e.g. play an important role for lattice paths in a strip, see [5,9]. It is nice that the other symmetric polynomials also have a combinatorial interpretation, as presented in the following table.

Let us now give a more formal definition of the corresponding objects and a proof of the formulas for the associated generating functions.

▶ **Definition 12.** *A positive meander is a path from $\ell \geqslant 0$ to $k \geqslant 0$ staying strictly above the x-axis (and possibly touching it at at most one of its end points). The generating function is denoted by $M^+_{\ell,k}(z)$. Negative meanders are defined similarly, with the condition to stay strictly below the x-axis.*

In Table 2, we focus on positive meanders from 0 to k and from k to 0. Note that it suffices to consider the paths from 0 to k as by time-reversion they are mapped to each other. In particular, let $u_i(z)$ and $v_j(z)$ be the small and large roots of the initial model. Then, after time-reversion the small roots are $\frac{1}{v_j(z)}$ and the large roots are $\frac{1}{u_i(z)}$. More details are given in the long version.

Table 2 In this article, we show that the fundamental symmetric polynomials (of the complete homogeneous, elementary, and power sum type) are counting families of positive meanders (walks touching the x-axis only at one of the end points and staying always above the x-axis). The functions $v_j(z)$ for $j = 1, \dots, d$ are the roots of the kernel equation $1 - zS(u) = 0$ with $\lim_{z=0} |v_j(z)| = +\infty$, whereas the functions $u_i(z)$ for $i = 1, \dots, c$ are the roots such that $\lim_{z=0} u_i(z) = 0$.

	from 0 to k	from k to 0
positive meander	 $M^{+}_{0,k}(z) = h_k\left(\frac{1}{v_1(z)}, \dots, \frac{1}{v_d(z)}\right)$	 $M^{+}_{k,0}(z) = h_k\left(u_1(z), \dots, u_c(z)\right)$
positive meander avoiding $(0,k)$	 $M^{\geqslant}_{0,k}(z) = (-1)^{k-1} e_k\left(\frac{1}{v_1(z)}, \dots, \frac{1}{v_d(z)}\right)$	 $M^{\geqslant}_{k,0}(z) = (-1)^{k-1} e_k\left(u_1(z), \dots, u_c(z)\right)$
positive meander marked below the minimum	 $M^{\bullet}_{0,k}(z) = p_k\left(\frac{1}{v_1(z)}, \dots, \frac{1}{v_d(z)}\right)$	 $M^{\bullet}_{k,0}(z) = p_k\left(u_1(z), \dots, u_c(z)\right)$

▶ **Theorem 13** (Generating function of positive meanders).

$$M^{+}_{0,k}(z) = h_k\left(\frac{1}{v_1(z)}, \dots, \frac{1}{v_d(z)}\right).$$

Proof. Observe that a meander ending at altitude k can be uniquely decomposed into an initial excursion followed by a positive meander from 0 to k. By [4, Theorem 2] their generating function is the coefficient of u^k in $\prod_{j=1}^{d} \frac{1}{1-u/v_j(z)}$. Consequently, by Equation (5) this is the generating function of the complete homogeneous symmetric polynomials $h_k(1/v_1(z), \dots, 1/v_d(z))$. ◀

This theorem gives a shorter proof of [4, Corollary 3]:

▶ **Corollary 14.** *The generating function $M_k(z)$ of meanders ending at altitude k are given by*

$$M_k(z) = E(z) h_k\left(\frac{1}{v_1(z)}, \dots, \frac{1}{v_d(z)}\right) = \frac{1}{s_d z} \sum_{\ell=1}^{d} \left(\prod_{j \neq \ell} \frac{1}{v_j(z) - v_\ell(z)}\right) \frac{1}{v_\ell(z)^{k+1}}.$$

Proof. As in the proof of Theorem 13, we use that positive meanders are classical meanders factored by excursions. Then a partial fraction decomposition of (5) yields the result. ◀

The last class we consider is the one of elementary symmetric polynomials. These are associated to a decorated class of paths.

▶ **Definition 15.** *A positive meander avoiding a strip of width k is a positive meander from 0 to k that always stays above any point of altitude $j < k$ except for its start point. The generating function is denoted by $M^{\geqslant}_{0,k}(z)$.*

▶ **Theorem 16** (Positive meanders avoiding the strip $[0, k]$)**.**

$$M^{\geqslant}_{0,k}(z) = (-1)^{k-1} e_k\left(\frac{1}{v_1(z)}, \dots, \frac{1}{v_d(z)}\right).$$

Proof. We proceed by induction on k. The base case $k = 1$ holds due to $M^{\geqslant}_{0,1}(z) = M^{+}_{0,1}(z) = 1/v_1(z) + \cdots + 1/v_d(z)$. Next assume the claim holds for $M^{\geqslant}_{0,1}(z), \dots, M^{\geqslant}_{0,k-1}(z)$.

Take an arbitrary positive meander from 0 to k. Either it is a positive meander avoiding the strip of width k, or at least one of its lattice points has an altitude smaller than k.

Let $0 < i < k$ be the altitude of the last step below altitude k. Then the path can be uniquely decomposed into an initial part from altitude 0 to this altitude i and a part from this point to the end. Note that by the construction the initial part starts at altitude 0 and then always stays above the x-axis, whereas the last part avoids a strip of width $k - i$. In terms of generating functions this gives

$$M^{\geqslant}_{0,k}(z) = M^{+}_{0,k}(z) - \sum_{i=1}^{k-1} M^{+}_{0,i}(z) M^{\geqslant}_{0,k-i}(z).$$

Inserting the known expressions, we get

$$M^{\geqslant}_{0,k}(z) = \sum_{i=1}^{k} (-1)^{k-i} e_{k-i}\left(\frac{1}{v_1}, \dots, \frac{1}{v_d}\right) h_i\left(\frac{1}{v_1}, \dots, \frac{1}{v_d}\right) = (-1)^{k-1} e_k\left(\frac{1}{v_1}, \dots, \frac{1}{v_d}\right),$$

thanks to the fundamental involution relation [38, Equation (7.13)] between elementary symmetric polynomials and complete homogeneous symmetric polynomials. ◀

▶ **Corollary 17.** *The generating functions of generalized arches (as introduced in Definition 4) satisfy (for $k > 0$)*

$$\begin{aligned} A_k &= \frac{(-1)^{k-c} s_{-c} z}{u_1(z) \cdots u_c(z)}\, e_k\left(\frac{1}{v_1(z)}, \dots, \frac{1}{v_d(z)}\right), \\ A_{-k} &= \frac{(-1)^{k-c} s_{-c} z}{u_1(z) \cdots u_c(z)}\, e_k\left(u_1(z), \dots, u_c(z)\right). \end{aligned}$$

Proof. This follows from $A_k = M^{\geqslant}_{0,k}/E$ and $A_{-k} = M^{\geqslant}_{k,0}/E$. ◀

We end our discussion with a third class of positive meanders.

▶ **Definition 18.** *A positive meanders marked below the minimum is a positive meander with an additional marker in $\{1, \dots, m\}$ where m is its minimal positive altitude. The generating function for such paths from 0 to k is denoted by $M^{\bullet}_{0,k}(z)$.*

For example it is immediate that $M^{\bullet}_{0,1}(z) = M^{\geqslant}_{0,1}(z) = M^{+}_{0,1}(z)$ as the only restriction is to avoid the x-axis. Furthermore, $M^{\bullet}_{0,0}(z) = 0$ while $M^{\geqslant}_{0,0}(z) = M^{+}_{0,0}(z) = 1$.

▶ **Theorem 19** (Positive meanders marked below the minimum).

$$M^{\bullet}_{0,k}(z) = p_k\left(\frac{1}{v_1(z)}, \ldots, \frac{1}{v_d(z)}\right).$$

Proof (Sketch). Every path from 0 to k has to touch at least one of the altitudes $1, \ldots, d$, as the largest possible up step is $+d$. We decompose any positive meander from 0 to k into two parts by cutting at the unique last positive minimum m. The first part is an arch avoiding the strip of width m, whereas the second part is a positive meander from m to k. Translating this decomposition into generating functions, we get

$$M^{\bullet}_{0,k}(z) = \sum_{m=1}^{d} m M^{\geqslant}_{0,m}(z) M^{+}_{0,k-m}(z),$$

where the factor m encodes the m possible ways to put a mark below the minimum, see Definition 18. Note that $M^{\geqslant}_{0,k}(z) = 0$ for $k > d$. Thus, by Theorems 13 and 16 we get

$$\sum_{k\geqslant 1} M^{\bullet}_{0,k}(z)u^k = \left(u\frac{\partial}{\partial u}\sum_{j\geqslant 0} M^{\geqslant}_{0,j}(z)u^j\right)\left(\sum_{i\geqslant 0} M^{+}_{0,i}(z)u^i\right) = \sum_{i=1}^{d}\frac{u/v_i(z)}{1-u/v_i(z)}.$$

By Equation (7) this proves the claim. ◀

5 Asymptotics and limit laws

We end the discussion on the symmetric polynomial expressions by deriving their respective asymptotics: this allows us to revisit some limit laws in which the appearance of symmetric polynomials was so far unrecognized.

We only consider *aperiodic* step sets $\mathcal{S}$, which are defined by $\gcd\{|i-j| : i, j \in \mathcal{S}\} = 1$. For the treatment of periodic step sets see [6]. We only treat paths from k to 0, as the formulas are a bit simpler. The results for paths from 0 to k follow in an analogous fashion. The principal small branch $u_1(z)$ and the principal large branch $v_1(z)$ are defined by the property that they are real positive for near $0+$ and meet at $z = \rho$; see [4].

In the next theorem we give the asymptotics of our three classes of positive meanders.

▶ **Theorem 20.** *Consider an aperiodic step set $\mathcal{S}$. Let τ be the structural constant determined by $S'(\tau) = 0$, $\tau > 0$. For the different variants of positive meanders given in Table 2, the number of paths from k to 0 of size n has the following asymptotic expansions*

$$[z^n]M^{+}_{k,0}(z) = \alpha_1\frac{S(\tau)^n}{2\sqrt{\pi n^3}}\left(1+\mathcal{O}\left(\frac{1}{n}\right)\right), \qquad \alpha_1 = \frac{\partial e_k}{\partial x_1}(\tau, u_2(\rho), \ldots, u_c(\rho)).$$

The number of positive meanders avoiding $(0,k)$ from k to 0 of size n satisfies

$$[z^n]M^{\geqslant}_{k,0}(z) = \alpha_2\frac{S(\tau)^n}{2\sqrt{\pi n^3}}\left(1+\mathcal{O}\left(\frac{1}{n}\right)\right), \qquad \alpha_2 = \frac{\partial h_k}{\partial x_1}(\tau, u_2(\rho), \ldots, u_c(\rho)).$$

The number of positive meanders marked below the minimum from k to 0 of size n satisfies

$$[z^n]M^{\bullet}_{k,0}(z) = \alpha_3\frac{S(\tau)^n}{2\sqrt{\pi n^3}}\left(1+\mathcal{O}\left(\frac{1}{n}\right)\right), \qquad \alpha_3 = \frac{\partial p_k}{\partial x_1}(\tau, u_2(\rho), \ldots, u_c(\rho)).$$

Proof. Let $\mathcal{M}_{k,0}^{+}$, $\mathcal{M}_{k,0}^{\geqslant}$, and $\mathcal{M}_{k,0}^{\bullet}$ be the sets of positive meanders, positive meanders avoiding $(0,k)$, and positive meanders marked below the minimum, respectively; see Table 2. Let $\omega_k \in \mathcal{A}_k$ and $\omega_{-k} \in \mathcal{A}_{-k}$ be two generalized arches. Now, define the multiset $\mathcal{E}_k$ that consists of d copies of the set $\{w : \omega_k \cdot w \in \mathcal{E}\}$ of excursions factored by ω_k. Then, the following chain of inclusions holds:

$$\mathcal{E} \cdot \omega_{-k} \subseteq \mathcal{M}_{k,0}^{\geqslant} \subseteq \mathcal{M}_{k,0}^{+} \subseteq \mathcal{M}_{k,0}^{\bullet} \subseteq \mathcal{E}_k. \tag{8}$$

The first inclusion holds as every walk $e \cdot \omega_{-k}$ with $e \in \mathcal{E}$ is a positive meander avoiding $(0,k)$. The middle inclusions hold by definition (see Table 2). The last inclusion holds since, for every $m \in \mathcal{M}_{k,0}^{\bullet}$, we have $\omega_k \cdot m \in \mathcal{E}$ after removing the marker from m. Therefore, the exponential growth rates of the counting sequences of $\mathcal{E} \cdot \omega_{-k}$ and $\mathcal{E}_k$ are equal to the one of classical excursions $\mathcal{E}$, which has been explicitly computed in [4]. Hence, all 3 classes of meanders in (8) have the same asymptotic growth R^n.

Next, we observe that the corresponding generating functions have non-negative coefficients, and whence Pringsheim's Theorem [22, Theorem IV.6] guarantees the existence of a dominant singularity on the positive real axis $\mathbb{R}^+$. By [4] this is the only dominant singularity and we have $\rho = 1/R$. Furthermore, it was shown that on the radius of convergence $|z| = \rho$ only one root $u_1(z)$ is singular and has a square-root singularity, while the other ones are analytic. Then, we combine this result with the explicit shape of the symmetric polynomials from Definition 11. This gives the Puiseux expansion at $z = \rho$ on which we apply singularity analysis to derive the claimed formulas. ◀

Before we continue, let us comment on an often overlooked phenomenon concerning the analyticity of the small branches.

▶ Remark 21 (Singularities of the small roots). The small roots (and, in particular the principal small branch $u_1(z)$) can have a singularity inside the disk of convergence of $E(z)$. For example, for $S(u) = u + 13/u + 6/u^2$, one easily checks that the radius of convergence of $E(z)$ is $\rho = 8/61$ while $u_1(z)$ and $u_2(z)$ are singular at $z = -1/8$. However, their product $u_1 u_2$ is regular for $|z| < \rho$; more generally what is proven in [4] is that the product of the small roots is always regular for $0 < |z| < \rho$, while in general not each single small root is regular for $0 < |z| < \rho$.

Many theorems leading to a Gaussian distribution require that a key quantity (let us call it σ) is nonzero. In [22], this nonzero assumption is called "variability condition"; see therein Theorem IX.8 (Quasi-power theorem), Theorem IX.9 (Meromorphic schema), Theorem IX.10 (Positive rational systems). Now, many lattice path statistics have a variance with an expansion $\sigma n + o(n)$, where σ is defined as in the following lemma, and is therefore nonzero.

▶ **Lemma 22** (Universal positivity of the variability condition). *For any Laurent series $S(u) = \sum_{i \geqslant -c} s_i u^i$, with $s_i \geqslant 0$ (at least two $s_i > 0$), one has $\sigma := S''(1)S(1) + S'(1)S(1) - S'(1)^2 > 0$.*

Proof. The trick is to introduce $\sigma(u) := uS''(u)S(u) + S'(u)S(u) - uS'(u)^2$. Then, all the monomials of $\sigma(u)$ have positive coefficients: this follows from $[s_i s_j]\sigma(u) = u^{i+j-1}(i-j)^2 \geqslant 0$, and thus $\sigma(u) > 0$ for $u > 0$. ◀

It is worth noting that an alternative version of this lemma is: « $uS(u)/S'(u) = n$ has no double root for $u > 0$ »; this plays a role in the tuning of Boltzmann random generation [17]. Such considerations are also related to Harald Cramér's trick of shifting the mean which transforms a problem with drift into a problem with zero drift, via the modification of the weights of the step set $\widetilde{S}(u) := S(\tau u)/S(\tau)$ (and choosing τ such that $S'(\tau) = 0$ indeed implies that $\widetilde{S}'(1) = 0$). Compare also with the proof of [21, Formula (2.37)].

As a consequence, Lemma 22 guarantees that we can apply the quasi-power theorem [22, Theorem IX.8], and obtain a Gaussian limit theorem. This explains why many statistics related to lattice paths are Gaussian. E.g., for paths with positive or zero drift, it furnishes a Gaussian limit theorem for the final altitude of meanders or for the height of walks. When the drift is negative, one gets some discrete limit laws of parameter given by our symmetric polynomial expressions:

▶ **Theorem 23** ([4, Theorem 6] and [41, Theorem 4.7]; negative drift cases)**.** *Assume a negative drift $\delta = S'(1) < 0$ and let $\rho = 1/P(\tau)$ and $\rho_1 = 1/P(1)$.*

1. *Let X_n be the random variable of the final altitude of a meander of length n. Then, the limit law is discrete and given by*

$$\lim_{n\to\infty} \Pr(X_n = k) = (1-\tau^{-1}) \frac{\sum_{i=0}^{k} \tau^{i-k} h_i(v_1(\rho)^{-1}, \dots, v_d(\rho)^{-1})}{\sum_{i\geqslant 0} h_i(v_1(\rho)^{-1}, \dots, v_d(\rho)^{-1})}.$$

2. *Let Y_n be the random variable of the height of a walk of length n. Then, the limit law is discrete and given by*

$$\lim_{n\to\infty} \Pr(Y_n = k) = \frac{h_k(v_1(\rho_1)^{-1}, \dots, v_d(\rho_1)^{-1})}{\sum_{i\geqslant 0} h_i(v_1(\rho_1)^{-1}, \dots, v_d(\rho_1)^{-1})}.$$

Proof (Sketch). Recall that for a path represented by a sequence of points $(\omega_0, \omega_1, \dots, \omega_n)$ the final altitude is ω_n and the height is $\max_i \omega_i$. In both cases the limit law follows from a rewriting of the closed form of the discrete probability generating function which basically consists of the generating function of h_k (alternatively, M^+) and proper rescaling. ◀

Note that the second case is an avatar of the Wiener–Hopf decomposition which links the height of walks with the final altitude of meanders; see Theorem 10 and [41].

6 Conclusion and perspectives

In this article we introduced the notion of prime walks, a class of walks which leads to natural decompositions of lattice paths and to concise proofs of several identities in probability theory that we are even able to further generalize by capturing some additional statistics. Moreover, these decompositions can keep track of some additional parameters (e.g. counting the number of occurrences of some given patterns, see [3]), which then gives access to many joint distribution studies, see e.g. [12].

Our work also offers new links with symmetric polynomials, adding to previous fundamental connections with algebraic combinatorics via Vandermonde determinants, the Jacobi–Trudi identity, and Schur functions (see [5, 9]). In [6], we give an interpretation of Schur polynomials (for some appropriate index) in terms of meanders ending at a given altitude. Together with the results of the present work, this extends the table given in [38, Prop. 2.8.3]: therein, Stanley gives some nice combinatorial expressions for the bases of symmetric functions (Definition 11), when they are evaluated at specific values like $x_i = 1$ or $x_i = q^i$. This is what he calls the "principal specializations". Our work shows that what we could call the "kernel root specialization" of the symmetric function bases (i.e. evaluation at $x_i = u_i(z)$) is leading to the enumeration of fundamental lattice path classes, holding for any set of jumps.

En passant, we illustrate the old Schützenberger philosophy: most of the identities in the commutative world are images of structural identities in the non-commutative world. It is natural to ask how far we can extend the link between lattice paths and the non-commutative symmetric world; note that further non-commutative points of view are developed in [18, 23, 24].

It is striking that astonishingly powerful formulas can be obtained by astonishingly simple tools from symbolic combinatorics. Such formulas, e.g. the Spitzer formula for bridges, have some unexpected avatars. Indeed, bridges of length n can be seen as $[u^0]S(u)^n$ for some Laurent polynomial $S(u)$ and the same holds with multivariate polynomials; this leads to some interesting connections between the non-commutative world, the Laurent phenomenon (i.e. the fact that some expressions which by design are a priori rational functions are in fact some Laurent polynomial), and lattice paths (see [14, 29, 36]).

On the computer algebra side, the so-called "Platypus algorithm" from [4] is a way to get the algebraic equation satisfied by the generating function of excursions. Another nice consequence of our formulas is that they permit a generalization of this "Platypus algorithm": starting from the generating functions of the symmetric polynomials given in Definition 11, we show in the long version of this article how to get the algebraic equations of the different families of constrained meanders, bridges, etc. This offers an effective alternative to an approach by resultants or Gröbner bases, which are quickly time and memory consuming.

For Motzkin paths (that is, paths with step set $\mathcal{S} = \{-1, 0, +1\}$), the generating functions associated to starting/final altitude constraints can be expressed as continued fractions, and thus as quotients of orthogonal polynomials [20]. Our work, in one sense, gives the generalization of these formulas as soon as one has steps $> +1$ or < -1. Many combinatorial structures related to the Motzkin paths have some asymptotics in which the "algebra of orthogonal polynomials" plays a role (e.g. the height of binary trees, related to the Mandelbrot fractal equation involves Chebyshev polynomials, see e.g. [22]). It is thus natural to ask if there is a nice "algebra of symmetric polynomials" in which plugging the Puiseux expansions offered by the kernel method could lead to the limit laws of many parameters of lattice paths?

In conclusion, our work largely complements and extends [4], being part of a wider program illustrating how lattice path surgery (which we call *latticepathology*) leads directly to many neat enumerative, probabilistic, computational, and asymptotic formulas.

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The Complexity of the Approximate Multiple Pattern Matching Problem for Random Strings

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Abstract

We describe a multiple string pattern matching algorithm which is well-suited for approximate search and dictionaries composed of words of different lengths. We prove that this algorithm has optimal complexity rate up to a multiplicative constant, for arbitrary dictionaries. This extends to arbitrary dictionaries the classical results of Yao [SIAM J. Comput. 8, 1979], and Chang and Marr [Proc. CPM94, 1994].

2012 ACM Subject Classification Theory of computation → Formal languages and automata theory; Theory of computation → Design and analysis of algorithms

Keywords and phrases Average-case analysis of algorithms, String Pattern Matching, Computational Complexity bounds

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.3

Funding *Andrea Sportiello*: Supported by the French ANR-MOST MetAConC.

1 The problem

1.1 Definition of the problem

Let Σ be an alphabet of s symbols, $\xi = \xi_0 \dots \xi_{n-1} \in \Sigma^n$ a word of n characters (the input *text string*), $D = \{w_1, \dots, w_\ell\}$, $w_i \in \Sigma^*$ a collection of words (the *dictionary*). We say that $w = x_1 \dots x_m$ occurs in ξ with final position j if $w = \xi_{j-m+1}\xi_{j-m+2} \cdots \xi_j$. We say that w occurs in ξ with final position j, with no more than k errors, if the letters $x_1, \dots, x_m$ can be aligned to the letters $\xi_{j-m'}, \dots, \xi_j$ with no more than k errors of insertion, deletion or substitution type, i.e., it has *Levenshtein distance* at most k to the string $\xi_{j-m'} \dots \xi_j$ (see an example in Figure 1). Let $r_m(D)$ be the number of distinct words of length m in D. We call $\boldsymbol{r}(D) = \{r_m(D)\}_{m \geq 1}$ the *content* of D, a notion of crucial importance in this paper.

The *approximate multiple string pattern matching problem* (AMPMP), for the datum (D, ξ, k), is the problem of identifying all the pairs (a, j) such that $w_a \in D$ occurs in ξ with final position j, and no more than k errors (cf. Figure 1). This is a two-fold generalisation of the classical *string pattern matching problem* (PMP), for which the exact search is considered, and the dictionary consists of a single word.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 3; pp. 3:1–3:15
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

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            5    10   15   20   25   30   35   40   45   50   55
        now.is.the.winter.of.our.discontent.made.glorious.summer
sour    ....................Xour.....................XouX.......
intent  ............inteXX...........Xntent.....................
galore  .........................................glorX..........
therein .......theSSin..........................................
```

soul: 23, 48;   intent: 16, 35;   galore: 45;   therein: 14.

Figure 1 Typical output of an approximate multiple string pattern matching problem, on an English text (alphabet of 26 characters plus the space symbol .). In this case $k = 2$ and $\boldsymbol{r}(D) = (0, 0, 0, 0, 1, 0, 2, 1, 0, \ldots)$. The symbols D, S and i stand for deletion, substitution and insertion errors, while X corresponds to an insertion or a substitution.

A precise historical account of this problem, and a number of theoretical facts, are presented in Navarro's review [8]. The first seminal works have concerned the PMP. Results included the design of efficient algorithms (notably Knuth–Morris–Pratt and Boyer–Moore), and have led to the far-reaching definition of the Aho–Corasick automata [1, 3, 7, 11]. In particular, Yao [11] is the first paper that provide rigorous bounds for the complexity of PMP in random texts. To make a long story short, it is argued that an interesting notion of complexity is the asymptotic average fraction of text that needs to be accessed (in particular, at least at this stage, it is *not* the time complexity of the algorithm), and is of order $\ln(m)/m$ for a word of length m. The first works on approximate search, yet again for a single word (APMP), are the description of the appropriate data structure, in [10, 4], and, more relevant to our aims here, the derivation of rigorous complexity bounds in Chang and Marr [5]. Yet again in simplified terms, if we allow for k errors, the complexity result of Yao is deformed into order $[\ln(m)+k]/m$. More recent works have concerned the case of dictionaries composed of several words, all of the same length [9],[1] however, also at the light of unfortunate flaws in previous literature, the rigorous derivation of the average complexity for the MPMP has been missing even in the case of words of the same length, up to our recent paper [2], where it is established that the Yao scaling $\ln(m)/m$ is (roughly) modified into $\max_m \ln(mr_m)/m$ (a more precise expression is given later on). By combining the formula of Chang and Marr for APMP, and our formula for MPMP, it is thus natural to expect that the AMPMP may have a complexity of the order $\max_m[\ln(mr_m) + k]/m$. This paper has the aim of establishing a result in this fashion.

Of course, the present work uses results, ideas and techniques already presented in [2], for the PMPM. A main difference is that in [2] we show that, for any dictionary, a slight modification of an algorithm by Fredriksson and Grabowski [6] is optimal within a constant, while this is not true anymore for approximate search with Levenshtein distance (we expect that it remains optimal for approximate search in which only substitution errors are allowed, although we do not investigate this idea here). As a result, we have to modify this algorithm more substantially, by combining it with the algorithmic strategy presented in Chang and Marr [5], and including one more parameter (to be tuned for optimality). This generalised algorithm is presented in Section 2.2.

Also, a large part of our work in [2] is devoted to the determination of a relatively tight lower bound, while the determination of the upper bound consists of a simple complexity analysis of the Fredriksson–Grabowski algorithm. Here, instead, we will make considerable

[1] This is the reason why, before our paper [2], which deals with dictionaries having words of different length, the forementioned notion of "content" of a dictionary did not appear in the literature.

Table 1 Summary of average complexities for exact and approximate search, for a single word or on arbitrary dictionaries. The results are derived from Yao [11], Chang and Marr [5], our previous paper [2], and the present paper, respectively.

	exact	approximate
single word	$C_{\text{Yao}} \dfrac{\ln m}{m}$ (Yao)	$C_{\text{CM}} \dfrac{\ln m + k}{m}$ (Chang and Marr)
dictionary	$C_1^{\text{ex}} \dfrac{1}{m_{\min}} + C_2^{\text{ex}} \max\limits_m \dfrac{\ln(smr_m)}{m}$	$\dfrac{C_1 k + C_1'}{m_{\min}} + C_2 \max\limits_m \dfrac{\ln(smr_m)}{m}$

efforts in order to determine an upper bound for the complexity of our algorithm, which is the content of Section 2.4, while we will content ourselves of a rather crude lower bound, derived with small effort in Section 1.3 by combining the results of [5] and [2].

1.2 Complexity of pattern matching problems

In our previous paper [2] we have established a lower bound for the (exact search) multiple pattern matching problem, in terms of the size s of the alphabet, and the content $\boldsymbol{r} = \{r_m\}$ of the dictionary, involving the length $m_{\min}$ of the shortest word in the dictionary, and a function $\phi(\boldsymbol{r})$ with the specially simple structure $\phi(\boldsymbol{r}) = \max_m f(m, r_m)$. More precisely, calling $\Phi_{\text{aver}}(\boldsymbol{r})$ (resp. $\Phi_{\max}(\boldsymbol{r})$) the average over random texts, of the average (res. maximum) over dictionaries D of content $\boldsymbol{r}$, of the asymptotic fraction of text characters that need to be accessed, we have

▶ **Theorem 1** (Bassino, Rakotoarimalala and Sportiello, [2]). *Let $s \geq 2$ and $m_{\min} \geq 2$, and define $\kappa_s = 5\sqrt{s}$. For all contents $\boldsymbol{r}$, the complexity of the MPMP on an alphabet of size s satisfies the bounds*

$$\frac{1}{\kappa_s}\left(\phi(\boldsymbol{r}) + \frac{1}{2s\, m_{\min}}\right) \leqslant \Phi_{\text{aver}}(\boldsymbol{r}) \leqslant \Phi_{\max}(\boldsymbol{r}) \leqslant 2\left(\phi(\boldsymbol{r}) + \frac{1}{2s\, m_{\min}}\right), \tag{1}$$

where

$$\phi(\boldsymbol{r}) := \max_m \frac{1}{m} \ln(s\, m\, r_m)\,. \tag{2}$$

Note a relative factor $\ln s$ between the statement of the result above, and its original formulation in [2], due to a slightly different definition of complexity.

As we have anticipated, such a result is in agreement with the result of Yao [11], for dictionaries composed of a single word, which is simply of the form $\ln(m)/m$. Combining this formula with the complexity result for APMP, derived in Chang and Marr [5], it is natural to expect that the AMPMP has a complexity whose functional dependence on k and $\boldsymbol{r}$ is as in Table 1. Indeed, the bottom-right corner of the table is consistent both with the entry above it, and the entry at its left. Furthermore, it is easily seen that, up to redefining the constants, several other natural guesses would have this same functional form in disguise. Let us give some examples of this mechanism. Write $X \gtrless a_{\text{L/U}} Y + b_{\text{L/U}} Z$ as a shortcut for $a_{\text{L}} Y + b_{\text{L}} Z \leqslant X \leqslant a_{\text{U}} Y + b_{\text{U}} Z$. Now, suppose that we establish that $\Phi(\boldsymbol{r}, k) \gtrless a_{\text{L/U}}\,(k+1)/m_{\min} + b_{\text{L/U}} \max_m (\ln(mr_m) + k)/m$. Then we also have $\Phi(\boldsymbol{r}, k) \gtrless a'_{\text{L/U}}\,(k+1)/m_{\min} + b_{\text{L/U}} \max_m \ln(mr_m)/m$, with $a'_{\text{U}} = a_{\text{U}} + b_{\text{U}}$ (and all other constants unchanged). On the other side, if we have $\Phi(\boldsymbol{r}, k) \gtrless a_{\text{L/U}}\,(k+1)/m_{\min} + b_{\text{L/U}} \max_m \ln(mr_m)/m$, with $a_{\text{L}} > b_{\text{L}}$, then we also have $\Phi(\boldsymbol{r}, k) \gtrless a_{\text{L/U}}\,(k+1)/m_{\min} + b'_{\text{L/U}} \max_m (\ln(mr_m) + k)/m$, with $b'_{\text{L}} = a_{\text{L}} - b_{\text{L}}$.

The precise result that we obtain in this paper is the following:

▶ **Theorem 2.** *For the AMPMP, with k errors and a dictionary D of content $\{r_m\}$, the complexity rate $\Phi(D)$ is bounded in terms of the quantity*

$$\widetilde{\Phi}(D) := \frac{C_1(k+1)}{m_{\min}} + C_2 \max_m \frac{\ln(smr_m)}{m} \tag{3}$$

as

$$\frac{1}{C_1 + \kappa_s C_2} \widetilde{\Phi}(D) \leqslant \Phi(D) \leqslant \widetilde{\Phi}(D)\,, \tag{4}$$

with $a = \ln(2s^2/(2s+1))$, $a' = \ln(4s^2-1)$, $\kappa_s = 5\sqrt{s}$ (as in Theorem 1) and

$$C_1 = \frac{a+2a'}{a}\,; \qquad C_2 = \frac{2(a+2a')}{aa'} = \frac{2}{a'} C_1\,. \tag{5}$$

1.3 The lower bound

Now, let us derive a lower bound of the functional form as in Table 1 for the AMPMP, by combining our results in [2] for the MPMP and the results in [5] for the APMP. Let us first observe a simple fact. Suppose that we have two bounds $A^{\mathrm{LB}}(\boldsymbol{r},k) \leqslant \Phi(\boldsymbol{r},k) \leqslant A^{\mathrm{UB}}(\boldsymbol{r},k)$ and $B^{\mathrm{LB}}(\boldsymbol{r},k) \leqslant \Phi(\boldsymbol{r},k) \leqslant B^{\mathrm{UB}}(\boldsymbol{r},k)$ (with $A^{\mathrm{LB}}(\boldsymbol{r},k)$ and $B^{\mathrm{LB}}(\boldsymbol{r},k)$ positive). Then, for all functions $p(\boldsymbol{r},k)$, valued in $[0,1]$, we have

$$p(\boldsymbol{r},k)A^{\mathrm{LB}}(\boldsymbol{r},k) + (1-p(\boldsymbol{r},k))B^{\mathrm{LB}}(\boldsymbol{r},k) \leqslant \Phi(\boldsymbol{r},k) \leqslant A^{\mathrm{UB}}(\boldsymbol{r},k) + B^{\mathrm{UB}}(\boldsymbol{r},k)\,.$$

We want to exploit this fact by using as bounds $A^{\mathrm{LB/UB}}(\boldsymbol{r},k)$ our previous result for the exact search, and as lower bound $B^{\mathrm{LB}}(\boldsymbol{r},k)$ the simple quantity $(k+1)/m_{\min}$. Then, later on, in Section 2, we will work on the determination of a bound $B^{\mathrm{UB}}(\boldsymbol{r},k)$ which has the appropriate form for our strategy above to apply. Let us discuss why $\Phi(\boldsymbol{r},k) \geq (k+1)/m_{\min}$. We will prove that this quantity is a bound to the minimal density of a *certificate*, over a single word of length $m = m_{\min}$, and text ξ. A certificate, as described in [11], is a subset $I \subseteq \{1,\dots,n\}$ such that, for the given text, the characters $\{\xi_i\}_{i \in I}$ imply that no occurrences of words of the dictionary may be possible, besides the ones which are fully contained in I. Some reflection shows that: (1) for the interesting case $m > k$, the smallest density $|I|/n$ of a certificate is realised on a *negative certificate*, that is, on a text ξ with no occurrences of the word w; (2) the smallest density is realised, for example, by the text $\xi = bbb\cdots b$, and the word $w = aaa\cdots a$; (3) in such a certificate, we must have read at least $k+1$ characters in every interval of size m, otherwise the alignment of w to this portion of text, in which we perform all the substitutions on the disclosed characters, would still be a viable candidate. Note in particular that deletion and insertion errors do not lead to higher lower bounds (although, for large m, they lead to bounds which are only slightly smaller).

As a result, recalling the expression for the lower bound in Theorem 1, by choosing $p(\boldsymbol{r},k)$ to satisfy $\frac{p}{1-p} = \frac{\kappa_s C_2}{C_1}$ we have

$$\Phi(\boldsymbol{r},k) \geq (1-p)\frac{k+1}{m_{\min}} + \frac{p}{\kappa_s}\phi(\boldsymbol{r}) = \frac{p}{\kappa_s C_2}\left(C_1 \frac{k+1}{m_{\min}} + C_2 \phi(\boldsymbol{r})\right) = \frac{C_1 \frac{k+1}{m_{\min}} + C_2\phi(\boldsymbol{r})}{C_1 + \kappa_s C_2}\,.$$

This proves the lower bound part of Theorem 2. Note that we could confine all the dependence from $\{r_m\}$ to the function ϕ (in particular, the choice $\frac{p}{1-p} = \frac{\kappa_s C_2}{C_1}$ only depends on the size of the alphabet s).

2 The (q, L) search algorithm, and the upper bound

2.1 Definition of alignment

We define a *partial alignment* α of the word $w = x_1 \dots x_m$ to the portion of text $\xi_{i_1} \dots \xi_{i_2}$, with k errors, and boundary parameters $(\varepsilon, \varepsilon') \in \mathbb{N}$, as the datum $\alpha = (w; i_1, i_2; \varepsilon, \varepsilon'; u)$, where u is a string in $\{C, S_a, D, I_a\}^*$, (these letters stand for *correct*, *substitution*, *deletion* and *insertion*, respectively, and the index a runs from 1 to s). Two integer parameters (for example i_2 and ε') are not independent, as they are deduced (say) from i_1, ε and the length of u. Indeed, say that the string u has m_C symbols C, m_D symbols D, m_S symbols of type S_a (for all a's altogether) and m_I symbols of type I_a, then

$$
\begin{aligned}
k &= m_S + m_D + m_I && \text{(number of errors)} \\
\varepsilon + \varepsilon' &= m - (m_C + m_S + m_D) && \text{(portion of the word on the sides)} \\
i_2 - i_1 + 1 &= m_C + m_S + m_I && \text{(length of the aligned portion of text)}
\end{aligned}
$$

The alignment has the following pattern (with a dash $-$ denoting a skipped character, in the text or in the word):

$$
\begin{array}{rc|ccccccccccc|c}
 & & i_1 & & & & & & & & & & i_2 & \\
\xi_{i_1} \cdots \xi_{i_2} = & \dots & \xi_{i_1} & \dots & w_j & \dots & \texttt{-} & \dots & a & \dots & a & \dots & \xi_{i_2} & \dots \\
u = & & & \dots & C & \dots & D & \dots & S_a & \dots & I_a & \dots & & \\
w = & \underbrace{w_1 \cdots w_\varepsilon}_{\varepsilon} & w_{\varepsilon+1} & \dots & w_j & \dots & w_{j'} & \dots & w_{j''} & \dots & \texttt{-} & \dots & w_{m-\varepsilon'} & \underbrace{w_{m-\varepsilon'+1} \cdots w_m}_{\varepsilon'}
\end{array}
$$

For example, if $w = \texttt{counteroffers}$, in our reference text of Figure 1 we have the alignment $\alpha = (w; i_1, i_2; \varepsilon, \varepsilon'; u) = (w; 14, 24; 3, 1; u)$ with $k = 4$ and $u = CCCCI_{\square}CCS_{\square}S_{\mathtt{o}}I_{\mathtt{u}}C$, as indeed

$$
\begin{array}{rrccccccccccccl}
 & & \underline{i_1} = 14 & & & & & & & & & & \underline{i_2} = 24 & & \\
\xi = & \cdots\texttt{the.wi} & \texttt{n} & \texttt{t} & \texttt{e} & \texttt{r} & \texttt{.} & \texttt{o} & \texttt{f} & \texttt{.} & \texttt{o} & \texttt{u} & \texttt{r} & & \texttt{.discontent}\cdots \\
u = & & C & C & C & C & I_{\square} & C & C & S_{\square} & S_{\mathtt{o}} & I_{\mathtt{u}} & C & & \\
w = & \underbrace{\texttt{cou}}_{\varepsilon = 3} & \texttt{n} & \texttt{t} & \texttt{e} & \texttt{r} & \texttt{-} & \texttt{o} & \texttt{f} & \texttt{f} & \texttt{e} & \texttt{-} & \texttt{r} & \underbrace{\texttt{s}}_{\varepsilon' = 1} &
\end{array}
$$

This example shows an important feature of this notion: several strings u may correspond to equivalent alignments among the same word and the same portion of text, and with the same offset ε. For example, the three last errors of $u = \cdots S_{\square}S_{\mathtt{o}}I_{\mathtt{u}}C$ can be replaced as in $u' = \cdots S_{\square}I_{\mathtt{o}}S_{\mathtt{u}}C$ or as in $u'' = \cdots I_{\square}S_{\mathtt{o}}S_{\mathtt{u}}C$. As the underlying idea in producing an upper bound from an explicit algorithm is to analyse the algorithm while using the union bound on the possible alignments, it will be useful to recognise classes of equivalent alignments, and, in the bound, "count" just the classes, instead of the elements (we are more precise on this notion in Section 2.3).

We define a *full alignment* to be likewise a partial alignment, but with $\varepsilon = \varepsilon' = 0$. That is, the goal of any algorithm for the AMPMP is to output the list of (say) positions i_2 of the full alignments among the given text and dictionary. Note that we can always complete a partial alignment with k errors and boundary parameters $(\varepsilon, \varepsilon')$ to a full alignment with no more than $k + \varepsilon + \varepsilon'$ errors, and no less than k errors, by including substitution or insertion errors at the two sides.

We define a *c-block partial alignment* as the generalisation of the notion of partial alignment to the case in which the portion of text consists of c non-adjacent blocks. In this case, besides the natural alignment parameters ε, ε', and $i_{1,a}$, $i_{2,a}$, and u_a, for the blocks

```
                    now.is.the.winter.of.our.discontent.made.glorious
                                     I□          D
deformed.pattern                 def ormed.pat-ten
                                     I□          Sn
                                 def ormed.pat-tern
```

Figure 2 Typical outcome for the search of the pattern `deformed pattern` in our reference text. In this example $L = 3$ and $q = 12$, the number of full blocks is $c(\alpha) = 2$, and can be aligned to the disclosed portion of the text (denoted by underline) with $k = 3$ errors: one deletion on the first block, one insertion in the second block, and one deletion somewhere in between the two blocks. On the bottom line, another alignment of the same word, in which, instead of inserting the letter `r` in the second block, we have substituted `n` by `r`, still with $k = 3$. These two alignments are sufficiently different to contribute separately to our estimate of the complexity, within our version of the union bound (because the values of ε are different).

$a = 1, \dots, c$, we have $c - 1$ parameters $\delta_a \in \mathbb{Z}$, associated to the offset between the alignment of the word to the blocks with index a and $a + 1$. As a result, in order to extend a c-block partial alignment to a full alignment, we need to perform at least $-\delta_a$ further insertion errors, or $+\delta_a$ further deletion errors, depending on the sign of δ_a, for each of the $c - 1$ intervals between the portions of text. That is, any c-block partial alignment α with k errors can be completed to a full alignment with no less than $k + \sum_a |\delta_a|$ errors.

Note that in the following we will *not* need to count all of the possible ways in which these deletions or insertions can be performed, as it may seem natural in a naïve perspective on the use of the union bound. This fact will allow us to efficiently bound the number of possible multi-block partial alignments arising in our algorithm analysis (instead of counting directly the possible full alignments, which would result in a too large bound).

2.2 The algorithm

Here we introduce an algorithm for AMPMP, concentrating on the pertinent notion of complexity, which is the ratio between the number of accesses to the text and the length of the text, and neglecting all implementation issues, and analysis of time complexity.

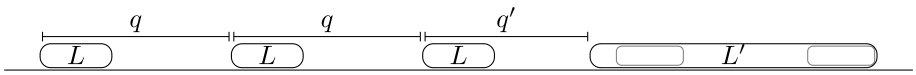
The algorithm is determined by two integers q and L, such that $k+1 \leqslant L < q \leqslant m_{\min} - k$. The emerging inequality $2k + 1 < m_{\min}$ is not a limitation, as when this inequality is not satisfied we have to read a fraction $\Theta(1)$ of the text, and in this regime there is no point in showing that some algorithm can reach a complexity which is optimal up to a multiplicatve constant. When $L = 1$, the algorithm coincides with the one described by Fredriksson and Grabowski [6], and already analysed in detail in [2] for the MPMP. When we have a single word of length m, and q has the maximal possible value $q = m - k$, the algorithm coincides with the one used by Chang and Marr [5] for their proof of complexity of the APMP. As we will see in Section 2.5, choosing the optimal values of q and L for a given dictionary D (when the words are of different length) is not a trivial task.

Call the interval $\xi_{bq}\xi_{bq+1} \cdots \xi_{bq+L-1}$ of the text ξ the *b-th block of text*. The text is thus decomposed in a list of blocks of length L, and of intervals between the blocks, of length $q - L$. To every possible full alignment α of the word w to the text, are associated two integers: $c(\alpha)$ is the number of blocks which are fully contained in the alignment, and $b(\alpha)$ is the index of the rightmost of these blocks. Furthermore, we define $c(w)$ as the minimum of $c(\alpha)$ among the possible alignments involving w (indeed, it is either $c(\alpha) = c(w)$ for all α, or $c(\alpha) \in \{c(w), c(w) + 1\}$ for all α, and, of course, at fixed q and L, $c(w)$ only depends on the length $|w|$ of the word).

Our algorithm accesses the text in three steps, namely, for every block index $b = 0, 1, \dots, \lceil n/q \rceil - 1$:

- We read all the characters ξ_i of the text, for $bq \leqslant i < bq + L$, that is we read the b-th block;
- We consider the possible c-block partial alignments α (with $c = c(\alpha)$) such that $b(\alpha) = b$, and associated to the intervals of text read so far. If any of these alignments is not excluded or determined positively, we read also the characters ξ_i for $i = bq - 1$, $bq - 2, \dots$, one by one, in this order, up to when all partial alignments are either excluded, or reach $\varepsilon = 0$. For a given instance of the problem, call $\mathcal{E}_L(b)$ (left-excess at block b) the set of positions of further characters that we need to access by this second step (with indices shifted so that the block starts at 1), and $e_L(b) = |\mathcal{E}_L(b)|$.
- If at the previous step we still have partial alignments which are not excluded, we read also the characters at positions $i = bq + L$, $bq + L + 1, \dots$, in this order, up to when all partial alignments are either excluded, or completed to a full alignment. Similarly to above, introduce $\mathcal{E}_R(b)$ and $e_R(b) = |\mathcal{E}_R(b)|$ (right-excess at block b).

An example with $c(\alpha) = 2$ is in Figure 2. Note that, at all steps, the pattern of the accessed part of the text consists of some blocks of length L and spacing q, plus one rightmost block with length $L' \geq L$ and spacing $q' \leqslant q$. A typical situation within the second step is as follows (here $c = 5$, $L = 3$, $q = 8$, $L' = 12$ and $q' = 7$):



Call $\mathcal{E}(b) = \mathcal{E}_L(b) \cup \mathcal{E}_R(b)$, and $e(b) = e_L(b) + e_R(b)$. Call Ψ_h^{exact} the average over random texts of the indicator function for the event that $e(b) \geq h$. Clearly, the average complexity rate of our algorithm is bounded by the expression

$$\Phi_{\mathrm{alg}}(D) \leqslant \frac{L + \mathbb{E}(e(b))}{q} = \frac{L + \sum_{h \geq 1} \Psi_h^{\mathrm{exact}}}{q} ,$$

where the average is taken over random texts, at fixed dictionary. Note that, because of our choice of range for q and L, $c(\alpha) \geq 1$ for all α, and $c(|w|) \geq 1$ for all w.

Let α be a full alignment associated to the block b. Call $\mathcal{E}[\alpha]$ the set of extra positions of the text (besides the blocks) that we need to access in order to determine the alignment α. Then clearly $\mathcal{E}(b) = \bigcup_\alpha \mathcal{E}[\alpha]$.

2.3 Proof strategy for the upper bound

Our proof strategy is to prove that there exists a choice of parameters L and q, with the properties that $q = \Theta(m_{\min})$, $L/q = \Theta(\phi(\boldsymbol{r}(D)))$, and $\mathbb{E}(e(b)) = \Theta(1)$. This last condition is equivalent to the requirement that Ψ_h^{exact} is a summable series, and we will see that indeed the first can be bounded by a geometric series, and the second is rather small. Up to calculating the pertinent multiplicative constants, such a pattern would imply the functional form of the complexity anticipated in Section 1.2.

The idea is that the exact calculation of $\mathbb{E}(e(b))$ or of Ψ_h^{exact}, even at q and L fixed (which is easier than optimising w.r.t. these parameters), is rather difficult, but we can produce a simpler upper bound by:

- For alignments α with $c(\alpha) > 1$, neglect the information coming from the $e(b')$ extra characters that we have accessed at blocks $b' < b$. This allows to separate the analysis on the different blocks of text.

- Naïvely, for different (full) alignments α, we could perform a *union bound*, that is, $e(b) = |\mathcal{E}(b)| = |\bigcup_\alpha \mathcal{E}[\alpha]| \leqslant \sum_\alpha |\mathcal{E}[\alpha]|$, which thus separates the analysis over the different alignments. We will make an improved version of this bound, namely we use this bound, not with full alignments, but rather with "classes of equivalent partial alignments".

As we anticipated, the crucial point is that we count partial alignments instead of full alignments. A further slight improvement of the bound comes from considering these 'classes of equivalent partial alignments', instead of just the partial alignments. These two facts are motivated by the same argument, that we now elucidate.

Consider the two following notions: (1) Each set $A_h(w)$ of partial alignments is partitioned into classes I. (2) There is a subset $\bar{A}_h(w) \subseteq A_h(w)$ of alignments, that we shall call *basic alignments*. Now, suppose that the two following properties hold: (i) $I \cap \bar{A}_h(w) \neq \varnothing$ for all classes I of $A_h(w)$. (ii) For each $\alpha \in I$, there exists a $\bar{\alpha} \in I \cap \bar{A}_h(w)$, such that $\mathcal{E}(\alpha) \subseteq \mathcal{E}(\bar{\alpha})$. In this case it is easily estalished that the bound above can be improved into $e(b) = |\mathcal{E}(b)| = |\bigcup_\alpha \mathcal{E}[\alpha]| \leqslant \sum_{\bar{\alpha}} |\mathcal{E}[\bar{\alpha}]|$, where the sum runs only on basic partial alignments. Thus, calling $\Psi_h := \sum_{w\in D} \sum_{\alpha \in \bar{A}_h(w)} \mathbb{P}(|\mathcal{E}[\bar{\alpha}]| \geq h)$, we have $\Psi_h \geq \Psi_h^{\text{exact}}$.

We propose the following definition of basic alignment. Let α be in $A_h(w)$. In the string u, suppose that we write C_a instead of C, whenever the well-aligned character is a, and D_a when the deleted character is a (this is clearly just a bijective decoration of u). For $\alpha \in \bar{A}_h(w)$, we require that there are no occurrences of $C_a I_a$ as factors of u (as these are equivalent to $I_a C_a$), of $C_a D_a$ (as these are equivalent to $D_a C_a$) and of $I_a D_b$ or $D_b I_a$ (as these are equivalent to C_a or S_a, depending if $a = b$ or not). If α can be obtained from α' by a sequence of these rewriting rules, then α and α' are in the same class I.

It is easy to see that this definition of basic alignment and classes has the defining properties above.

2.4 Evaluation of an upper bound at q and L fixed

Let us call $p_{c,h,\varepsilon'}(w)$ the probability that, for a given word w and parameter ε', there exists an alignment $\alpha \in A_h(w)$, to a text consisting of $c-1$ blocks of length L and one block of length $L+h$, which is visited by the algorithm (that is, it makes at most k errors), that is, in particular,

$$\Psi_h \leqslant \sum_{\varepsilon'=0}^{q-1} p_{c,h,\varepsilon'}(w)\,. \tag{6}$$

We have the important fact

▶ **Proposition 3.**

$$p_{c,h,\varepsilon'}(w) \leqslant \beta s^{-(cL+h)} B_{cL+h+c-1,k} \tag{7}$$

for all ε', *where* $\beta = \frac{(2s-1)L+k}{(2s-1)L-k}$ *and* $B_{L,k} = (2s-1)^k \binom{L+k}{k}$.

The proof of this proposition is slightly complicated, and is presented in Appendix A. Note however that for the special case $c = 1$, and with exactly k errors (instead of at most k errors), the bound $s^{-(L+h)}(2s)^k \binom{L+k}{k}$ can be established trivially. Also note that the bound does not depend on ε', and, in particular, it only depends on $h = |\mathcal{E}_L| + |\mathcal{E}_R|$ for the alignments α at given w and ε', and not separately on the two summands.

We are now ready to evaluate the expressions for the upper bound on the quantity Ψ_h in (6), in light of (7). Call $R_c = \sum_{m\,:\,c(m)=c} r_m = \sum_{m=qc+L-1}^{q(c+1)+L-2} r_m$, and $p_{c,h}$ as q times the RHS of (7) (that is, an upper bound to $\sum_{\varepsilon'=0}^{q-1} p_{c,h,\varepsilon'}(w)$). We have the bound

$$\sum_h \Psi_h \leqslant \sum_c R_c \sum_h p_{c,h} = \sum_c R_c \sum_h \beta\, q\, s^{-(cL+h)} B_{cL+h+c-1,k}\,. \tag{8}$$

Recalling that

$$\sum_{h\geq 0} s^{-h}\binom{a+k+h}{k} \leqslant \frac{1}{1-\frac{1}{s}\frac{a+k+1}{a+1}}\binom{a+k}{k},$$

(and that $q < m_{\min}$), substituting in (8) gives

$$\begin{aligned}\Phi_{\text{alg}}(D) &\leqslant \frac{1}{q}\left(L+\beta q\sum_c R_c \frac{1}{1-\frac{1}{s}\frac{cL+k+c}{cL+c}} s^{-cL}\binom{cL+c-1+k}{k}(2s-1)^k\right)\\ &\leqslant \frac{1}{q}\left(L+\frac{\beta m_{\min}(2s-1)^k}{1-\frac{1}{s}\frac{L+k}{L}}\sum_c R_c\, s^{-cL}\binom{c(L+1)+k}{k}\right). \end{aligned} \tag{9}$$

We want to prove that

$$\Phi_{\text{alg}}(D) \leqslant \frac{C_1 k + C_1'}{m_{\min}} + C_2 \max_m \frac{\ln(smr_m)}{m}, \tag{10}$$

with suitable constants C_1, C_1' and C_2 (it will turn out at the end that we can set $C_1' = C_1$ and C_1, C_2 to be as in Theorem 2, but at this point it is convenient to let them be three separate variables). This would prove the upper bound part of Theorem 2.

Note that, if $k/m_{\min} \geq 1/C_1$, the upper bound expression (10) is larger than the trivial bound $\Phi_{\text{alg}}(D) \leqslant 1$, and there is nothing to prove. So we can assume that $k/m_{\min} < 1/C_1$.

2.5 Optimisation of q and L

We now have to analyse the expression (9), in order to understand which values of q and L make the bound smaller. The sum over c is the most complicated term. We simplify it by using the fact that, for all $\xi \in \mathbb{R}^+$, $\ln\binom{a+k}{k} \leqslant k\ln(1+\xi) + a\ln(1+\xi^{-1})$, which gives

$$\begin{aligned} T &:= m_{\min}(2s-1)^k \sum_c R_c\, s^{-cL}\binom{c(L+1)+k}{k}\\ &\leqslant \sum_c \frac{1}{c^2}\exp\Big[-c\Big(LA - \frac{1}{c}\left(\ln(R_c m_{\min}) + k\ln((1+\xi)(2s-1))\right) - \frac{\ln c^2}{c} - \ln(1+\xi^{-1})\Big)\Big]\\ &= \sum_c \frac{1}{c^2}\exp\left[-c(LA - \phi'(c) - \ln(1+\xi^{-1}))\right], \end{aligned} \tag{11}$$

where $A = \ln(s\xi/(1+\xi))$, $A' = \ln((1+\xi)(2s-1))$ and

$$\phi'(c) = \frac{\ln(c^2 R_c m_{\min}) + kA'}{c}. \tag{12}$$

Ultimately, we want to choose L such that T is bounded by a constant, as its summands over c are bounded by a convergent series. With this goal, let c^* be the value maximising the expression $\phi'(c)$, and ϕ^* the value of the maximum. The sum above is then bounded by

$$\sum_c \frac{1}{c^2}\exp[-c(LA - \phi^* - \ln(1+\xi^{-1}))].$$

For any value of ξ such that $A > 0$ (that is, for $\xi > (s-1)^{-1}$), there exists a positive smallest value of L such that the exponent in the expression above is negative. So we set

$$L^* = \left\lceil \frac{\phi^* + \ln(1+\xi^{-1})}{A} \right\rceil,$$

(as the choice of ξ is free, we can tune it at the end so that the ratio is an integer), and recognise that the RHS of equation (11), specialised to $L = L^*$, is bounded by $\sum_c \frac{1}{c^2} = \pi^2/6$. Note that

$$\phi^* \geq \phi'(1) \geq kA'$$

so that

$$\frac{L^*}{k} \geq \frac{A'}{A} = \frac{\ln((1+\xi)(2s-1))}{\ln(s\,\xi/(1+\xi))},$$

which implies that we can set $\beta = \frac{2s-1+A/A'}{2s-1-A/A'}$, and

$$\frac{1}{1-\frac{1}{s}\frac{L+k}{L}} \leqslant \frac{1}{1-\frac{1}{s}(1+A/A')} = \frac{1}{1-\frac{1}{s}\frac{\ln(s\xi(2s-1))}{\ln((1+\xi)(2s-1))}}.$$

Now, let us choose $q = \lfloor \frac{m_{\min}-k}{2} \rfloor$, which coincides with the choice of the analogous parameter in Chang and Marr [5]. This is the largest possible value such that $c(w) \geq 1$ for all $w \in D$. With this choice,

$$\frac{1}{q} \leqslant \frac{2}{m_{\min}} \frac{C_1}{C_1 - 1}.$$

Collecting the various factors calculated above, we get that the expression (9) is bounded by

$$\Phi_{\mathrm{alg}}(D) \leqslant \frac{2}{m_{\min}} \frac{C_1}{C_1-1} \left(L^* + \frac{\beta \frac{\pi^2}{6}}{1-\frac{1}{s}(1+A/A')} \right).$$

We are left with two tasks: choosing suitable values for ξ and C_1 (both of order 1), and recognising that the expression for L^* (and for ϕ^*) can be related to the quantity $\phi(\boldsymbol{r})$ in (2). Let us start from the latter. Note that, as for any $m \geq m_{\min}$

$$\frac{m-k}{q} - 2 \leqslant c(m) \leqslant \frac{m}{q}$$

we can write[2] $m \leqslant m_{\min} c(m) \leqslant s^2 m$, which gives

$$\max_c \frac{1}{c} \ln(c^2 m_{\min} R_c) \leqslant \max_m \frac{m_{\min}}{m} \ln(s^2 m^2 r_m) \leqslant 2 m_{\min} \phi(\boldsymbol{r}).$$

As, of course $\max_c (X(c) + Y(c)) \leqslant \max_c X(c) + \max_c Y(c)$, we have in particular that

$$\phi^* \leqslant 2 m_{\min} \phi(\boldsymbol{r}) + kA' \qquad\qquad L^* \leqslant \frac{2 m_{\min} \phi(\boldsymbol{r}) + kA' + \ln(1+\xi^{-1})}{A},$$

which thus implies

$$\begin{aligned}
\Phi_{\mathrm{alg}}(D) &\leqslant \frac{2}{m_{\min}} \frac{C_1}{C_1-1} \left(\frac{2m_{\min}}{A}\phi(\boldsymbol{r}) + k\frac{A'}{A} + \frac{\beta\frac{\pi^2}{6}}{1-\frac{1}{s}(1+A/A')} + \frac{\ln(1+\xi^{-1})}{A} \right) \\
&= \frac{2C_1}{C_1-1} \left[\frac{A'}{A} \frac{k}{m_{\min}} + \left(\frac{\beta\frac{\pi^2}{6}}{1-\frac{1}{s}(1+\frac{A}{A'})} + \frac{\ln(1+\xi^{-1})}{A} \right) \frac{1}{m_{\min}} + \frac{2}{A}\phi(\boldsymbol{r}) \right].
\end{aligned}$$

---

[2] Because $s \geqslant 2$, and we anticipate that, under our choice, $C_1 \geq 5$, thus

$$m \leqslant 2(m-k-q) \leqslant m_{\min} \left(\frac{m-k}{q} - 2 \right) \leqslant m_{\min} c(m) \leqslant m_{\min} \frac{m}{q} \leqslant 2 \left(\frac{C_1}{C_1-1} \right) m \leqslant s^2 m.$$

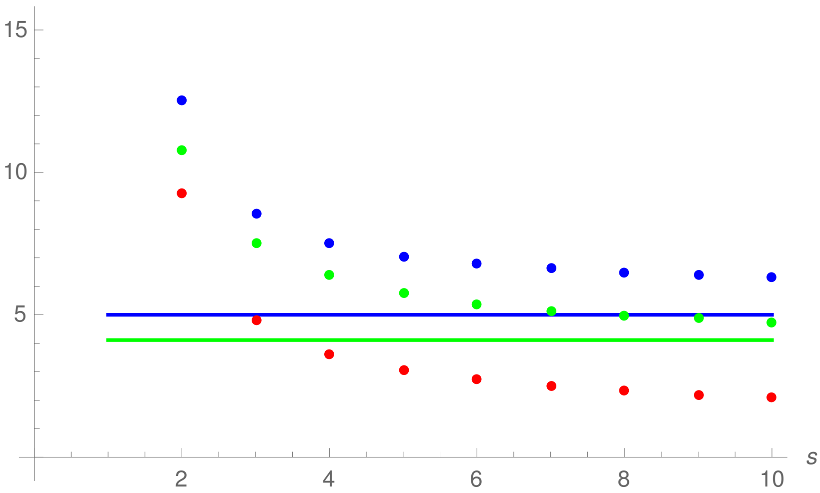


Figure 3 Plot of the constant $C_1(s)$, $C'_1(s)$ and $C_2(s)$, as given by the expressions in (13) (respectively, in blue, green and red). The asymptotic values are 5, $5\pi^2/12$ and 0 respectively.

Let us choose $C_1 = 2A'/A + 1$. The expression above simplifies into

$$\Phi_{\text{alg}}(D) \leqslant \frac{C_1 k}{m_{\min}} + \frac{2A' + A}{AA'} \left[\left(\frac{A\beta\frac{\pi^2}{6}}{1 - \frac{1}{s}(1 + \frac{A}{A'})} + \ln(1 + \xi^{-1}) \right) \frac{1}{m_{\min}} + 2\phi(\boldsymbol{r}) \right] ,$$

in particular, this justifies the notation C_1, which in the introduction was chosen to denote the coefficient in front of the $\frac{k}{m_{\min}}$ summand. Now we shall choose the optimal value of ξ. The dependence on ξ is mild, provided that we are in the appropriate range $\xi > 1/(s-1)$. The choice of ξ, in turns, determines the ratio between the lower and upper bound, which has the functional form $C'_1 + \kappa_s C_2$ (with notations as in the theorem). A choice which is a good trade-off among the three summands in this expression, and for which the analytic expression is relatively simple, is to take $\xi = 2s$. Under this choice we have

$$C_1 = 1 + 2\frac{\ln(4s^2 - 1)}{\ln(2s^2/(2s+1))} , \qquad C_2 = \frac{4}{\ln(2s^2/(2s+1))} + \frac{2}{\ln(4s^2-1)} ,$$
$$C'_1 = \frac{C_2}{'2} \left[\ln\frac{2s+1}{2s} + \frac{\beta\pi^2}{6} \frac{s\ln(2s^2/(2s+1))\ln(4s^2-1)}{(s-1)\ln(4s^2-1) - \ln(2s^2/(2s+1))} \right]$$

or, in a more compact way, calling $a = A|_{\xi=2s} = \ln(2s^2/(2s+1))$ and $a' = A'|_{\xi=2s} = \ln(4s^2-1)$, and substituting back the value of β,

$$C_1 = \frac{a + 2a'}{a} , \qquad C_2 = \frac{a+2a'}{a}\frac{2}{a'} , \tag{13a}$$

$$C'_1 = \frac{a+2a'}{a}\left(\frac{\ln s - a}{a'} + \frac{\pi^2}{6}\frac{(2s-1)a' + a}{(2s-1)a' - a}\frac{as}{(s-1)a' - a} \right). \tag{13b}$$

The behaviour in s of these constants is depicted in Figure 3.

It can be verified that, with our choice of ξ, $C'_1 < C_1$ for all $s \geq 2$.[3] we can replace C'_1 by C_1 in the functional form (10) for the bound on $\Phi_{\text{alg}}(D)$, and thus obtain the statement of Theorem 2. This concludes our proof.

[3] One way to see this is by proving that both $C_1(s)$ and $C'_1(s)$ decrease monotonically as functions on the real interval $[2, +\infty[$, that $\lim_{s\to\infty} C_1(s) = 5$, that $C_1(s) > C'_1(s)$ for $s \in \{2, 3, \ldots, 7\}$, and that $C'_1(8) < 5$.

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A Proof of Proposition 3

In this section we evaluate an upper bound to $p_{c,h,\varepsilon'}$, which is the probability that, for a given word w with $c(|w|) = c$, the disclosed text composed of $c-1$ intervals of size L and one interval of size $L+h$ corresponds to at least one basic alignment α by making no more than k errors. The statement of the result, equation (14) below, is given in Proposition 3.

Let us introduce the recurring quantity

$$B_{L,k} := (2s-1)^k \binom{L+k}{k}.$$

First, let us analyse the case in which we have a single block, and exactly k errors. For w a word of length m, it is clear that the result depends only on the $m-\varepsilon'$ left-most characters of the word, not on the ε' right-most ones, so we can assume without loss of generality that $\varepsilon' = 0$. Call $H_{L,k}(m)$ the number of different words of length L obtained by transforming the suffixes of w and making exactly k errors. We have

▶ **Proposition A.1.** *For all $L \geq k \geq 1$, $H_{L,k} \leqslant B_{L,k}$.*

Proof. Note that the analogous statement with $2s-1$ replaced by $2s$ in $B_{L,k}$ is trivial, as we have exactly $2s$ types of errors (one deletion, s insertions and $s-1$ substitutions), and the counting of their possible positions in the string u is a function of the length of the string, bounded from above by the worst case, associated to all insertion errors.

We can gain the factor $2s-1$ instead of $2s$ by restricting to basic alignments, but this requires a finer analysis involving generating functions. Let us call $f(u, y, z)$ the generating function such that $[u^a y^L z^k]f(u, y, z)$ is the number of basic alignments of length L obtained by transforming a word of length a and making exactly k errors. Calculating $f(u,y,z)$ exactly is a difficult task, and the result would depend on w as a word, not only on $m = |w|$, but we will calculate a simpler upper bound $f_{\mathrm{UB}}(u,y,z)$, which in particular only depends on m. In this context, a generating-function upper bound is an upper bound for partial sums, that is $g \succeq f$ if $\sum_{h=0}^{k}[u^a y^L z^h](g(u,y,z) - f(u,y,z)) \geq 0$ for all L and a. Let us construct f_{UB} by starting from $f_0(u,y,z) := \frac{uy}{1-uy}$, which is the generating function f specialised to $z = 0$, and let us introduce the various types of errors one at the time.

The first operation corresponds to allow for *insertion* errors. The restriction to basic alignments, however, brings to a subtlety. For example, starting with a word $w = abcd$, in order to get the alignment $aaabcd$ we can proceed in several ways: $a\boldsymbol{aa}bcd$ or $\boldsymbol{aa}abcd$ or by $\boldsymbol{a}a\boldsymbol{a}bcd$ (bold letters correspond to insertions). Under the notion of basic alignment we avoid to overcount these manifestly equivalent alignments, as of these expressions we would only keep the latter, $\boldsymbol{aa}abcd$, that is, at the left of a letter a we can only insert letters different from a. On the other hand, at the right end of the word one can insert strings consisting of any character of the alphabet.

Calling f_i the generating function in which insertion errors are allowed, we thus get

$$f_i(u,y,z) = \frac{1}{1-syz} f(u,y,z)|_{uy \to uy\left(\frac{1}{1-(s-1)z}\right)} = \frac{uy}{(1-syz)(1-uy-(s-1)yz)}\,.$$

We now introduce deletion errors, which, consistently, we allow only on the characters of the initial string (not on the ones which have just been insterted). Thus, any given original character can be either left as is, or deleted. This gives the generating function $f_{i,d}$, with

$$f_{i,d}(u,y,z) = f_i(u,y,z)|_{uy \to uy+uz} = \frac{uz+uy}{(1-syz)(1-uy-uz-(s-1)yz)}\,.$$

Finally, for substitution errors, again we can either substitute any initial character with one of the $s-1$ other characters of the alphabet, or leave it unchanged, which brings to $f_{i,d,s}$, with

$$f_{i,d,s} = f_{i,d}(u,y,z)|_{uy \to uy+(s-1)uyz} = \frac{u(syz-yz+y+z)}{(1-syz)(1-uz-(s-1)(u+1)yz)}\,.$$

Note that, by this procedure, we have already produced an upper bound, as $f_{i,d,s} \succeq f$ (in the sense defined above). Note also that it is *not* $f_{i,d,s} = f$, because, for example, we have overcounted the equivalent cases in which in a word $w = \cdots aa \cdots$ we have deleted the first *or* the second character.

If the word w is shorter than $L+k$, we may miss some alignments because they do not fit in the text interval. As we are evaluating an upper bound, we can restrict to the case in which w is long enough for this not to happen, and thus sum over all suffixes by just setting $u = 1$, and conclude that $H_{L,k} \leqslant [y^L z^k] f'(1,y,z)$. Thus, in order to conclude, we must show that $[y^L z^k] f'(1,y,z) \leqslant B_{L,k}$. Let us call

$$F_{L,k} = [y^L z^k] \frac{1}{(syz-1)(2syz-2yz+y+z-1)}\,.$$

We can rewrite the inequality above as $H_{L,k} \leqslant F_{L-1,k} + F_{L,k-1} + (s-1)F_{L-1,k-1}$, and thus, if we can prove that $F_{L,k} \leqslant B_{L,k}$, for all pairs of integers $L \geqslant k$, we could conclude in light of the fact that

$$H_{L,k} \leqslant B_{L-1,k} + B_{L,k-1} + (s-1)B_{L-1,k-1} = (2s-1)^k \binom{L+k}{k} - R_{L,k}\,,$$

where $R_{L,k} = (2s-1)^{k-1}\left(2(s-1)\frac{k-1}{L}\binom{L+k-2}{k-1}\right)$ is indeed easily checked to be non-negative for all $L \geqslant k \geqslant 1$.

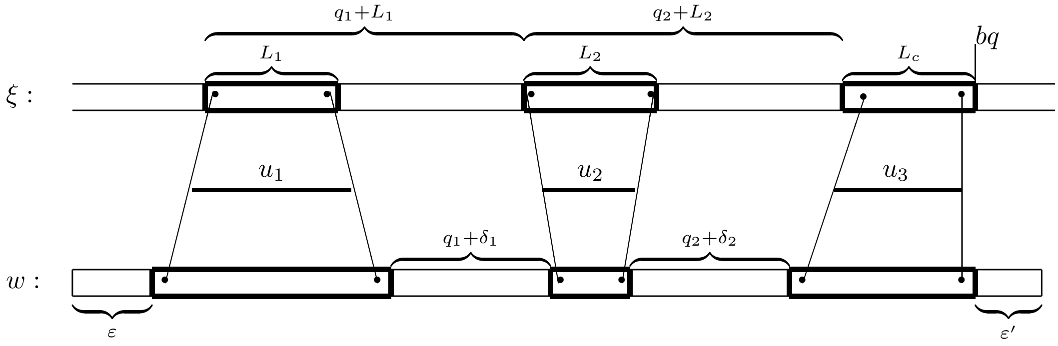

Figure 4 Example of multi-interval alignment analysed for the estimate of $p_{L_1,\dots,L_c;k}$.

So, to finish the proof, let us show that $F_{L,k} \leqslant B_{L,k}$. First,

$$F_{L,k} = [y^L z^k]\left(\frac{1}{1-syz} + \frac{2syz-2yz+y+z}{1-2syz+2yz-y-z}\right)$$
$$= \delta_{L,k}s^k + F_{L-1,k} + F_{L,k-1} + 2(s-1)F_{L-1,k-1}\,.$$

Since $L \geqslant k \geqslant 1$, we have $R_{L,k} \geqslant \delta_{L,k}s^k$ for $s \geqslant 2$, and $B_{L,k} \geqslant F_{L,k} \geqslant H_{L,k}$.

To conclude, we just check the boundary conditions in the recursion above for $F_{L,k}$ and $B_{L,k}$, which again are in agreement with the inequality. Indeed we have, for $(L,k) \in \{(0,0),(0,1),(1,0)\}$, $F_{0,0} = B_{0,0} = 1$, $B_{0,1} = 2s-1 \geq 1 = F_{0,1}$ and $B_{1,0} = 4s-2 \geq 3s = F_{1,0}$. ◀

Now we want to deal with the more general case, in which we have more than one block, and we sum over the number of errors up to k. We will prove a more general statement, in which we have c blocks of lengths $L_1, \dots, L_c$, separated by gaps of lengths $q_1, \dots, q_{c-1}$, which in particular is so general to allow us to treat in one stroke the case in which we add characters at the left or at the right of the b-th algorithm block.

Similarly to the argument above, in order to produce an upper bound we can set without loss of generality that $\varepsilon' = 0$, all the q_i's are larger than k and that m is larger than $\sum L_i + \sum q_i + k$, as any variant of this would give no more alignments. So, we will call $p_{L_1,\dots,L_c;k}$ the corresponding quantity, in which the dependence from the q_i's and m has been dropped.

For multi-block partial alignments, we have parameters $\delta_1, \dots, \delta_{c-1}$ for the offset among the different consecutive blocks of the partial alignment, and, if we have an offset δ_i in the alignment of two blocks, we have to perform at least $|\delta_i|$ deletions or insertions errors when completing the partial alignment to a full one (cf. figure 4).

Calling $\bar{L} = \sum_{i=1}^{c} L_i$, this leads to the following sum

$$p_{L_1,\dots,L_c;k} \leqslant s^{-\bar{L}} \sum_{t=0}^{k} \sum_{\Delta=0}^{t} \sum_{\substack{k_1,k_2,\dots,k_c \in \mathbb{N} \\ k_1+k_2+\dots+k_c = t-\Delta}} \sum_{\substack{\delta_1,\delta_2,\dots,\delta_{c-1} \in \mathbb{Z} \\ \delta_1+\delta_2+\dots+\delta_{c-1} = \Delta}} B_{L_1,k_1} B_{L_2,k_2} \dots B_{L_c,k_c}\,.$$

From the Vandermonde convolution formula, $\sum_{i=0}^{k} \binom{l_1+i}{i}\binom{l_2+k-i}{k-i} = \binom{l_1+l_2+k+1}{k}$, which implies $\sum_h B_{L_1,h} B_{L_2,k-h} = B_{L_1+L_2+1,k}$, we can simplify the expression above into

$$p_{L_1,\dots,L_c;k} \leqslant s^{-\bar{L}} \sum_{t=0}^{k} \sum_{\Delta=0}^{t} \sum_{\substack{\delta_1,\delta_2,\dots,\delta_{c-1} \in \mathbb{Z} \\ \delta_1+\delta_2+\dots+\delta_{c-1} = \Delta}} B_{\bar{L}+c-1,t-\Delta}\,.$$

The sum over the δ_i's gives

$$\sum_{\substack{\delta_1,\delta_2,\ldots,\delta_{c-1}\in\mathbb{Z}\\ \delta_1+\delta_2+\ldots+\delta_{c-1}=\Delta}} 1 = [z^{\Delta}]\left(\frac{1+z}{1-z}\right)^{c-1}$$

that is, by recognising that $B_{L,k-h} \leqslant B_{L,k}\left(\frac{k}{(2s-1)L}\right)^h$, we get

$$p_{L_1,\ldots,L_c;k} \leqslant s^{-\bar{L}} B_{\bar{L}+c-1,k}\left(\frac{(1+z)^{c-1}}{(1-z)^c}\right)\Bigg|_{z=\frac{k}{(2s-1)(\bar{L}+c-1)}}.$$

This is all we shall say at this level of generality. Now note that, in our patterns, $\bar{L}+c-1 \geq cL$ (and $k \leqslant L$), so that, in this range of parameters,

$$p_{L_1,\ldots,L_c;k} \leqslant s^{-\bar{L}} B_{\bar{L}+c-1,k}\left(\frac{(1+z)^{c-1}}{(1-z)^c}\right)\Bigg|_{z=\frac{1}{(2s-1)c}\frac{k}{L}} \leqslant \frac{(2s-1)+\frac{k}{L}}{(2s-1)-\frac{k}{L}} s^{-\bar{L}} B_{\bar{L}+c-1,k}\,. \tag{14}$$

Two Arithmetical Sources and Their Associated Tries

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Abstract

This article is devoted to the study of two arithmetical sources associated with classical partitions, that are both defined through the mediant of two fractions. The Stern-Brocot source is associated with the sequence of all the mediants, while the Sturm source only keeps mediants whose denominator is "not too large". Even though these sources are both of zero Shannon entropy, with very similar Renyi entropies, their probabilistic features yet appear to be quite different. We then study how they influence the behaviour of tries built on words they emit, and we notably focus on the trie depth.

The paper deals with Analytic Combinatorics methods, and Dirichlet generating functions, that are usually used and studied in the case of good sources with positive entropy. To the best of our knowledge, the present study is the first one where these powerful methods are applied to a zero-entropy context. In our context, the generating function associated with each source is explicit and related to classical functions in Number Theory, as the ζ function, the double ζ function or the transfer operator associated with the Gauss map. We obtain precise asymptotic estimates for the mean value of the trie depth that prove moreover to be quite different for each source. Then, these sources provide explicit and natural instances which lead to two unusual and different trie behaviours.

2012 ACM Subject Classification Theory of computation → Pattern matching; Theory of computation → Randomness, geometry and discrete structures

Keywords and phrases Combinatorics of words, Information Theory, Probabilistic analysis, Analytic combinatorics, Dirichlet generating functions, Sources, Partitions, Trie structure, Continued fraction expansion, Farey map, Sturm words, Transfer operator

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.4

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 4; pp. 4:1–4:19
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

Funding Laboratory IRP SINFIN, Projects DynA3S and CoDys (French ANR), Project AleaEnAmSud (STICAmSud), Projet RIN Alenor (Regional Project from French Normandy)
Eda Cesaratto: Partially supported by Universidad Nacional de General Sarmiento Grant 30/3307.
Martín D. Safe: Partially supported by Universidad Nacional del Sur Grant PGI 24/L115.

1 Introduction

A source is a way of producing random words from a given alphabet (see Definition 1). We study two arithmetical sources, each of them being associated with a classical family of partitions. These two families are defined through the mediant $(a+b)/(c+d)$ of the two fractions a/b and c/d. The first one, the Stern-Brocot source, is defined with the sequence of all the mediants, whereas the second one, the Sturm source, only keeps mediants whose denominator is "not too large". Even though the probabilistic features of the two sources appear to be quite different, they are both of zero Shannon entropy and their Renyi entropies appear to be quite similar. In Information Theory contexts, the trie structure built on words emitted by the source is a powerful tool for comparing words emitted by a source, and the shape of the trie – notably the average length of a branch, called the depth – can be viewed as a "measure" of the quality of the source. We then may expect that the trie depth behaves in a different way for each source, and provides a tool which strongly differentiates the two sources.

The probabilistic behaviour of the depth D_n of a trie built on n independent infinite words emitted by simple sources (memoryless and Markov sources) has been largely studied (see the book by Szpankowski [20] for a complete review in this case). In the context of "good" dynamical sources (with an entropy $\mathcal{E} > 0$) introduced in [23], the average-case analysis was first developed in [5], and [11], then a distributional analysis that exhibits a limit Gaussian law for D_n was performed in [4]. In all cases, for $n \to \infty$, the asymptotic mean value $\mathbb{E}[D_n]$ is of logarithmic order and involves the entropy, with the estimate $\mathbb{E}[D_n] \sim (1/\mathcal{E}) \log n$. The moments $\mathbb{E}[D_n^k]$ are proven to be of order $\Theta(\log^k n)$.

For sources of zero entropy, and to the best of our knowledge, the analysis of trie depth has not yet been performed in a general context. We study here the two arithmetical sources, associated with classical partitions, that have been previously presented. We obtain two results. First, for the two sources, all the moments of order $k \geq 2$ of the trie depth D_n behave in a similar way, as they are all infinite. However, the mean value $\mathbb{E}[D_n]$ exhibits a strong difference between the two sources, as $\mathbb{E}[D_n]$ is of order $\Theta(\log^2 n)$ for the Stern-Brocot source, and of order $\Theta(\sqrt{n})$ for the Sturm source.

Plan of the paper. Section 2 recalls the general context of sources, and focuses on the Analytic Combinatorics point of view. It introduces the two sources, and provides expressions for their Dirichlet generating functions (DGF's). Section 3 is devoted to tries, and focuses on the trie depth. It also presents the main analytical tool, the Rice formula, whose application is based on the tameness of the DGF's. Section 4 proves the tameness of DGF's in the two cases, and states the main result.

2 Sources, partitions, Dirichlet generating functions

We first recall two definitions of sources, and introduce the generating functions. We explain their roles in the analysis, notably for good sources. We then present the two sources of interest, with their DGF, and explain why the various notions of entropies are essentially the same for the two sources.

2.1 Sources and partitions

We first give a definition of a source, as it appears in Information Theory contexts.

▶ **Definition 1.** *A* probabilistic source $\mathcal{S}$ *over the finite (ordered) alphabet* $\Sigma := [0..r-1]$ *is a sequence* $Y := (Y_0, Y_1, \ldots, Y_i, \ldots)$ *of random variables* Y_i *with values in* Σ.

The value of the random variable Y_i is the symbol emitted by the source at the discrete time $t = i$, and the value of the sequence $Y \in \Sigma^{\mathbb{N}}$ is the (infinite) word emitted by the source.
Consider a finite word $w \in \Sigma^\star$, and denote by p_w the probability that Y begins with the prefix w. The set $(p_w)_{w\in\Sigma^\star}$ is called the set of *fundamental probabilities*, and the set $(p_w)_{w\in\Sigma^k}$ is the set of fundamental probabilities of *depth* k. We moreover assume

$$\pi_k := \max\{p_w \mid w \in \Sigma^k\} \text{ tends to } 0 \text{ as } k \to \infty\,.$$

With Kolmogorov's extension theorem, the probabilistic source defines a probability $\mathbb{P}$ on the space $\Sigma^{\mathbb{N}}$ which is completely specified by the set $(p_w)_{w\in\Sigma^k}$ of fundamental probabilities.

There are particular instances of sources that are defined via a family of (labelled) partitions. We first recall this notion.

▶ **Definition 2.** *A family* $(\mathcal{P}_k)_{k\geq 0}$ *of labelled partitions associated with the alphabet* $\Sigma := [0..r-1]$ *is built in a recursive way as follows.*

(*i*) *One begins with* $\mathcal{P}_0 = \{[0,1]\}$ *and we let* $\mathcal{I}_\varepsilon := [0,1]$

(*ii*) *For each* $k \geq 0$, *the partition* $\mathcal{P}_{k+1}$ *is a refinement of the partition* $\mathcal{P}_k$.

(a) $\mathcal{P}_{k+1}$ *arises from* $\mathcal{P}_k$ *by dividing each (closed) interval of* $\mathcal{P}_k$ *into* r *(closed) intervals using* $r-1$ *points of the interval.*

(b) *Each interval of* $\mathcal{P}_k$ *is a closed interval labelled as* $\mathcal{I}_w$ *with* $w \in \Sigma^k$ *and gives rise to* r *closed intervals that are labelled from the left to the right as* $\mathcal{I}_{w\cdot a}$ *with* $a \in \Sigma$.

(c) *The diameter* $\delta(\mathcal{P}_k) := \max\{|\mathcal{I}_w| \mid w \in \Sigma^k\}$ *tends to 0 for* $k \to \infty$.

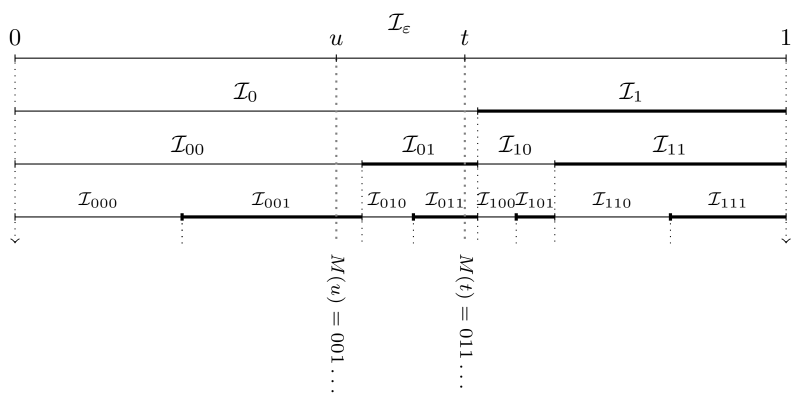


Figure 1 Example of a source defined via a family of partitions.

One now associates with this family $(\mathcal{P}_k)_{k\geq 0}$ of partitions a mapping $M : [0,1] \to \Sigma^{\mathbb{N}}$ that is defined outside the set $\mathcal{D}$ that gathers all the end-points of the intervals, as follows.
If $u \notin \mathcal{D}$, there exists, indeed, for each $k \geq 0$, a unique interval of $\mathcal{P}_k$ which contains (in its interior) the real u. Such an interval is labelled with a prefix $w \in \Sigma^k$. This prefix depends on the depth k and the real u, and is denoted as $w_k(u)$. As the partition $\mathcal{P}_{k+1}$ is a refinement of $\mathcal{P}_k$, and the diameter $\delta(\mathcal{P}_k) \to 0$, this sequence $w_k(u)$ of finite prefixes converges to a unique infinite word over the alphabet Σ that defines the value at u of the mapping M. (See Fig. 1).

In this way, the interval $\mathcal{I}_w$ gathers (up to a denumerable set) the reals u for which the word $M(u)$ begins with the prefix w. This is the fundamental interval of the prefix w, and its length is exactly the probability that $M(u)$ begins with w. Then, the mapping M defines a probabilistic source, whose fundamental probabilities are $p_w := |\mathcal{I}_w|$.

The paper deals with two instances of such a framework, over the binary alphabet $\Sigma := \{0, 1\}$. In both cases, the end-points of the partition are rational numbers, and the point which is added in the interval $[a/c, b/d]$ is the mediant $(a + b)/(c + d)$. It is always added in the first case, and gives rise to the Stern-Brocot partition. It is only added in the second case when its denominator is not too large: this partition is then defined via the Farey sequence, and, labelled in a convenient way, gives rise to what we call the Sturm partition.

2.2 Generating functions

Following the analytic combinatorics principles described in [10], and the main ideas introduced in [23], we associate, with a complex variable s, and a source, various Dirichlet generating functions (DGF's); first, $\Lambda_k(s)$ is relative to a given depth $k \geq 0$; second, $\Lambda(s)$ is associated with all possible depths; third, $\Lambda(s, v)$ is the bivariate generating function where the variable v "marks" the depth:

$$\Lambda_k(s) := \sum_{w\in\Sigma^k} p_w^s\,, \qquad \Lambda(s) := \sum_{w\in\Sigma^\star} p_w^s = \sum_{k\geq 0}\Lambda_k(s)\,, \qquad \Lambda(s,v) := \sum_{k\geq 0} v^k\Lambda_k(s)\,. \tag{1}$$

The bivariate DGF $\Lambda(s, v)$ proves very useful, due to the identity[1] $\Lambda_k(s) = [v^k]\Lambda(s, v)$ which possibly leads to use of singularity analysis.

All the main objects of a source that appear in a general Information Theory context – entropies, coincidence, trie parameters – are expressed with these series, as it is shown in [23] and [5], and now recalled: *Entropies* are the first classical parameters that describe the probabilistic properties of a source. They are defined with the DGF $\Lambda_k(s)$.

$$\text{[Shannon entropy]} \qquad \mathcal{E} = \lim_{k\to\infty} (1/k)\,\mathcal{E}_k, \qquad \mathcal{E}_k := \sum_{w\in\Sigma^k} p_w|\log p_w| = -\Lambda_k'(1)\,. \tag{2}$$

$$\text{[Renyi entropies of depth } k \text{ and exponent } \sigma > 1] \qquad \frac{1}{1-\sigma}\,\log\Lambda_k(\sigma)\,. \tag{3}$$

The *coincidence* between n words emitted by the source is defined as the length of their largest common prefix. Then, when the n words are independently drawn from the source, the coincidence becomes a random variable C_n defined on $[\Sigma^{\mathbb{N}}]^n$ whose distribution $\Pr[C_n \geq k + 1]$ exactly coincides with $\Lambda_k(n)$ and expectation $\mathbb{E}[C_n]$ coincides with $\Lambda(n)$.

The present paper mainly deals with another characteristic of the source, the *trie-depth*, denoted by D_n, which is expressed with the DGF $\Lambda(s)$, as recalled in (8).

2.3 A detour: review on the results for good sources

As it will be proven in Section 2.6, the two sources of interest are of zero entropy. They thus provide instances of sources that do not have the same behaviour as "good" sources, for instance memoryless sources or (ergodic) Markov Chains. Dynamical systems associated with expanding surjective maps of the interval provide other instances of "good" sources.

[1] As usual, the notation $[v^k]A(v)$ denotes the coefficient of v^k in $A(v)$.

We then recall (in a quite informal way) the main properties of the DGF's in the case of "good" sources. The DGF $\Lambda(s)$ is tame at $s = 1$ of order 1 (in the sense of Definition 9). Furthermore, there exists a basic function $s \mapsto \lambda(s)$, attached to each source, that is analytic on a neighborhood of the real axis $\Re s > d$ (for some $d < 1$, possibly equal to $-\infty$), and satisfies $\lambda(1) = 1$. This mysterious function is just equal to the sum $\sum_{i=0}^{r-1} p_i^s$ in the memoryless case. In the Markov chain case, this is the dominant eigenvalue of the matrix $P_s := (p_{i|j}^s)$ that extends the transition matrix P_1. Finally, in the case of ergodic dynamical sources, this is the dominant eigenvalue of the secant transfer operator $\mathbf{G}_s$ of the system.
The DGF's $\Lambda(s, v)$ and $\Lambda(s)$ essentially behave as quasi-inverses, for s close to the real axis,

$$\Lambda(s, v) \approx (1 - v\lambda(s))^{-1}, \qquad \Lambda(s) \sim_{s\to 1} (1 - \lambda(s))^{-1} \sim_{s\to 1} \frac{-1}{\lambda'(1)} \frac{1}{s-1}\,.$$

With properties of the bivariate DGF $\Lambda(s, v)$ and singularity analysis, the function $\Lambda_k(s)$ is a k-th quasi-power for s close to the real axis, and

$$\Lambda_k(s) = [v^k]\Lambda(s, v) \sim a(s)\lambda(s)^k \qquad (k \to \infty), \qquad \text{in particular} \quad \mathcal{E} = -\lambda'(1)\,.$$

These results, valid for "good" sources, will be used as comparison references in the rest of the paper. We now focus on the analysis of the two sources presented in the end of the Section 2.1 and obtain nice expressions for the DGF's described in Propositions 3 and 4.

2.4 The Stern-Brocot source

The *Stern-Brocot partition* of depth k, denoted as $\mathcal{B}_k$, is defined recursively as follows:

(i) One begins with $\mathcal{B}_0 = \{[0/1, 1/1]\}$;

(ii) For each $k \geq 1$, $\mathcal{B}_k$ arises from $\mathcal{B}_{k-1}$

by dividing each interval $[a/c, b/d]$ of $\mathcal{B}_{k-1}$ by its mediant $(a + b)/(c + d)$.

We now recall the relation between this family of partitions and the Farey map

$$T : [0, 1] \to [0, 1], \quad T(x) = x/(1-x) \;\text{ for } x \in [0, 1/2]\,, \quad T(x) = (1-x)/x \;\text{ for } x \in [1/2, 1]\,.$$

The set of the inverse branches of T is $\mathcal{H} := \{a, b\}$ with

$$a : [0, 1] \to [0, 1/2], \quad a(x) = x/(1 + x)\,; \qquad b : [0, 1] \to [1/2, 1], \quad b(x) = 1/(1 + x)\,;$$

Then, the set $\mathcal{H}^k := \{a, b\}^k$ of inverse branches of the iterate T^k generates the partition $\mathcal{B}_k$, and the set $\mathcal{B}_k$ gathers the fundamental intervals of depth k of the Farey map,

$$\mathcal{B}_k = \{[h(0), h(1)] \mid h \in \mathcal{H}^k\}.$$

The secant transfer operator $\mathbf{H}_s$ of the Farey map, defined as the sum $\mathbf{H}_s = \mathbf{A}_s + \mathbf{B}_s$, with

$$\mathbf{A}_s[G](x, y) := \left|\frac{a(x) - a(y)}{x - y}\right|^s G(a(x), a(y)),$$
$$\mathbf{B}_s[G](x, y) := \left|\frac{b(x) - b(y)}{x - y}\right|^s G(b(x), b(y))\,,$$

provides, via its iterates, the following expressions for the DGF's of the Stern-Brocot source,

$$\Lambda_k(s) = \mathbf{H}_s^k[1](0, 1) \quad \text{for } k \geq 0, \qquad \Lambda(s, v) = (I - v\mathbf{H}_s)^{-1}[1](0, 1)\,.$$

The decomposition $\mathcal{H}^\star = \{a^\star b\}^\star \cdot a^\star$ leads to the analogous decomposition for the quasi-inverse $(I - v\mathbf{H}_s)^{-1}$, namely $(I - v\mathbf{H}_s)^{-1} = (I - v\mathbf{A}_s)^{-1}(I - v\mathbf{B}_s(I - v\mathbf{A}_s)^{-1})^{-1}$.

For any $m \geq 1$, the LFT [2] $a^{m-1} \circ b$ coincides with the LFT $g_m : x \mapsto 1/(m+x)$ which is an inverse branch of the Gauss map. Then, the operator $v\mathbf{B}_s \circ (I - v\mathbf{A}_s)^{-1}$ coincides with a weighted version $\mathbf{G}_{s,v}$ of the secant transfer operator $\mathbf{G}_s$ of the Euclid DS, namely,

$$\mathbf{G}_{s,v}[F](x,y) := \sum_{m \geq 1} v^m \left| \left(\frac{1}{m+x} \right) \left(\frac{1}{m+y} \right) \right|^s F\left(\frac{1}{m+x}, \frac{1}{m+y} \right),$$

and coincides at $v = 1$ with the secant transfer operator $\mathbf{G}_s$. We have proven:

▶ **Proposition 3.** *The DGF's of the Stern-Brocot source satisfy*

$$\Lambda(s,v) = (I - v\mathbf{H}_s)^{-1}[1](0,1) = (I - v\mathbf{A}_s)^{-1}(I - \mathbf{G}_{s,v})^{-1}[1](0,1)\,;$$
$$\Lambda(s) = (I - \mathbf{H}_s)^{-1}[1](0,1) = (I - \mathbf{A}_s)^{-1}(I - \mathbf{G}_s)^{-1}[1](0,1)\,.$$

2.5 The Sturm source

We consider the source, called the Sturm source, which emits the Sturm characteristic words. More precisely, for each $\alpha \in [0,1]$, it emits the characteristic Sturm word $S(\alpha)$, whose definition is now recalled. Consider α of the interval $[0,1]$, the two intervals $I_0(\alpha) = [1-\alpha, 1[$ and $I_1(\alpha) = [0, 1-\alpha[$ it defines, together with the Kronecker-Weyl sequence $n \mapsto \{n\alpha\}$ (where $\{x\}$ denotes the fractional part of x). By definition, the n-th symbol of the word $S(\alpha)$ equals $j \in \{0,1\}$ if and only if $\{(n+1)\alpha\}$ belongs to $I_j(\alpha)$.

The partition $\mathcal{S}_k$ associated with the Sturm source of order k is defined by its end-points, that are the elements of the Farey sequence of depth $k+1$,

$$\mathcal{F}_{k+1} := \{\tfrac{a}{c} \mid a, c \geq 1,\ \gcd(a,c) = 1,\ c \leq k+1\}.$$

The partition $\mathcal{S}_k$ is built from $\mathcal{S}_{k-1}$ in a similar recursive way as the Stern-Brocot partition $\mathcal{B}_k$ is built from $\mathcal{B}_{k-1}$:

(i) One begins with $\mathcal{S}_0 = \mathcal{B}_0 = \{[0/1, 1/1]\}$

(ii) For each $k \geq 1$, $\mathcal{S}_k$ arises from $\mathcal{S}_{k-1}$

by dividing each interval $[a/c, b/d]$ of $\mathcal{S}_{k-1}$ by its mediant $(a+b)/(c+d)$ *provided the denominator $c+d$ be at most $k+1$.*

Due to the previous condition, the partition $\mathcal{S}_k$ is thus a pruning of the partition $\mathcal{B}_k$, and satisfies two classical properties

(P1) For any k, for any interval $[a/c, b/d]$ of $\mathcal{S}_k$, one has $ad - bc = -1$.

(P2) The set $\mathcal{C}_k$ which gathers the pairs (c,d) which appear as denominators of the intervals $[a/c, b/d] \in \mathcal{S}_{k-1}$ is equal to

$$\mathcal{C}_k := \{(c,d) \mid \max(c,d) \leq k < c+d, \quad \gcd(c,d) = 1\}\,.$$

Moreover, each pair (c,d) appears at most once. Then, the partition $\mathcal{S}_k$ has a polynomial number of intervals [of order $O(k^2)$] whereas the partition $\mathcal{B}_k$ has exactly 2^k intervals.

We now describe how to encode the partition $\mathcal{S}_k$ with the prefixes of length k of characteristic Sturmian words. The prefix of length k of the word $S(\alpha)$, denoted as $[S(\alpha)]_k$, satisfies two properties, described in [2, Proposition 3]:

(i) The two words $0 \cdot [S(\alpha)]_k$ and $1 \cdot [S(\alpha)]_k$ are both factors of the infinite word $S(\alpha)$;

(ii) For an interval $[a/c, b/d] \in \mathcal{S}_k$ with $a/c \neq 0$ and $b/d \neq 1$, one has the characterization

$$\forall \alpha \in]a/c, b/d[, \qquad [S(\alpha)]_k \ \text{ is a palindrome} \Longleftrightarrow c+d = k+2\,.$$

$\mathcal{S}_0 : (0)$						ε						(1)
$\mathcal{S}_1 : (0)$			0			$(1/2)$			1			(1)
$\mathcal{S}_2 : (0)$		00		$(1/3)$	01	$(1/2)$	10	$(2/3)$		11		(1)
$\mathcal{S}_3 : (0)$	000	$(1/4)$	001	$(1/3)$	010	$(1/2)$	101	$(2/3)$	110	$(3/4)$	111	(1)

Figure 2 The coding of the partition $\mathcal{S}_k$ for $k \leq 3$.

This property is used as follows for the coding of the partition $\mathcal{S}_k$: We begin with the coding of $\mathcal{S}_0$ as the empty word ϵ. Then, there are two cases: when the mediant can be added, the interval is subdivided and the coding of the two sub-intervals is made in the usual way, in the lexicographic order. When the mediant cannot be added, the interval is not subdivided, and its new coding is obtained in a unique way with a palindromic completion. (See Fig. 2)

We now study the generating functions.

▶ **Proposition 4.** *The generating series of the Sturm source can be expressed with double zeta functions $\zeta(a, b)$ together with the usual zeta function $\zeta(a)$ in the form*

$$\Lambda(s) = 1 + 2\frac{\zeta(s, s-1)}{\zeta(2s-1)} \qquad \textit{with} \quad \zeta(a) := \sum_{c \geq 1} \frac{1}{c^a}, \qquad \zeta(a, b) := \sum_{c \geq 1} \frac{1}{c^b} \sum_{d | d > c} \frac{1}{d^a}. \tag{4}$$

Proof. With Property $(P1)$, the length of an interval $[a/c, b/d] \in \mathcal{S}_k$ encoded by w, is equal to $p_w = 1/(cd)$. With $(P2)$, and the set $\mathcal{C}_k$ defined there, one obtains

$$\Lambda_{k-1}(s) = \sum_{(c,d) \in \mathcal{C}_k} \left(\frac{1}{cd}\right)^s, \qquad \Lambda(s) = \sum_{\substack{(c,d) \\ \gcd(c,d)=1}} \left(\frac{1}{cd}\right)^s \sum_{k \geq 0} [\![(c, d) \in \mathcal{C}_k]\!],$$

where $[\![\cdot]\!]$ is Iverson's bracket. Then,

$$\Lambda(s) = \sum_{\substack{(c,d) \\ \gcd(c,d)=1}} \left(\frac{1}{cd}\right)^s [(c + d) - \max(c, d)] = \sum_{\substack{(c,d) \\ \gcd(c,d)=1}} \frac{\min(c, d)}{(cd)^s}.$$

As the general term of the previous sum is homogeneous of weight $1 - 2s$, the two sums – the sum relative to general pairs (c, d) and the sum relative to coprime pairs – are related. The denominator $\zeta(2s - 1)$ appears, and, with the equality

$$\sum_{(c,d)} \frac{\min(c, d)}{c^s d^s} = \zeta(2s - 1) + 2\zeta(s, s - 1),$$

this yields the expression given in (4). ◀

The long version of the paper will provide an expression of the bivariate Sturm DGF $\Lambda(s, v)$ in terms of polylogarithms.

[2] LFT = linear fractional transformation

2.6 Entropies

The Shannon entropy defined in (2) is the first parameter associated with a source.

▶ **Proposition 5.** *The two sources are of zero Shannon entropy.*

Proof. (a) This is clear for the Sturm source. Jensen's inequality applied to the concave map $\phi(t) = t|\log t|$ relates $\mathcal{E}_k$ and the number A_k of (non empty) fundamental intervals of depth k, via the inequality $\mathcal{E}_k \le \log A_k$. One has indeed:

$$\frac{\mathcal{E}_k}{A_k} = \frac{1}{A_k} \sum_{\boldsymbol{w} \in \Sigma^k} \phi(p_w) \le \phi\left(\frac{1}{A_k} \sum_{w \in \Sigma^k} p_w\right) = \phi\left(\frac{1}{A_k}\right) = \frac{\log A_k}{A_k}, \quad \text{and thus} \quad \mathcal{E}_k \le \log A_k \,.$$

Then a source for which A_k is polynomial has a zero entropy. This applies to the Sturm source for which $A_k = O(k^2)$.

(b) This is also the case for the Stern-Brocot source. However, we do not find any direct proof of this fact in the literature. This is why we provide two proofs in the annex. ◀

The Renyi entropies of depth k and exponent $\sigma > 1$, defined via $\Lambda_k(\sigma)$ in (3), are already studied in at least two papers: The first result, due to Moshchevitin and Zhigljavsky in [16] describes the Stern-Brocot case. The second one, due to Hall [13] and Kanemitsu et al, describes in [14] the Sturm case.

▶ **Proposition 6.** [16, 13, 14] *As $k \to \infty$, the following asymptotic estimates hold for the DGF's $\Lambda_k(\sigma)$,*

$$[\text{Stern-Brocot case}, \sigma > 1] \qquad \Lambda_k(\sigma) = \frac{2}{k^\sigma} \frac{\zeta(2\sigma - 1)}{\zeta(2\sigma)} \left[1 + O\left(\frac{\log k}{k^{(\sigma-1)/(2\sigma)}}\right)\right] ; \tag{5}$$

$$[\text{Sturm case}, \sigma \ge 4] \qquad \Lambda_k(\sigma) = \frac{2}{k^\sigma} \frac{\zeta(\sigma - 1)}{\zeta(\sigma)} \left[1 + O\left(\frac{1}{k}\right)\right] . \tag{6}$$

The previous estimates for the two sources are then quite similar, with the same polynomial behaviour in $O(1/k^\sigma)$ for $k \to \infty$. Even though the dominant constants are not the same, they are however of the same spirit.

We then study another parameter of the source, the trie-depth, with the hope that it may "differentiate" the two sources in a stronger way.

3 Tries built from words emitted by a source

The trie structure is an important data structure in algorithmics [12] that also plays a central role in Theoretical Information Theory contexts. This is why it has already been deeply analyzed, at least in the context of good sources. See [20] for analyses in the context of simple sources and [5, 11, 4] for analyses in the context of dynamical sources.

3.1 Trie and its depth

A trie is a tree structure, used as a dictionary, which compares words emitted by a source $\mathcal{S}$ via their prefixes. The trie $\mathcal{T}(\boldsymbol{x})$ is built on a finite sequence $\boldsymbol{x}$ of (infinite) words emitted by the source $\mathcal{S}$ and is defined recursively by the following three rules which involve the cardinality $N(\boldsymbol{x})$ of the sequence $\boldsymbol{x}$:

(a) If $N(\boldsymbol{x}) = 0$, then $\mathcal{T}(\boldsymbol{x}) = \emptyset$

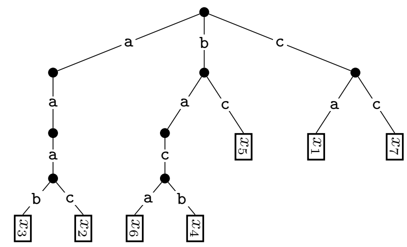
(b) If $N(\boldsymbol{x}) = 1$, with $\boldsymbol{x} = (x)$, then $\mathcal{T}(\boldsymbol{x})$ is a leaf labeled by x.

(c) If $N(\boldsymbol{x}) \geq 2$, then $\mathcal{T}(\boldsymbol{x})$ is formed with an internal node and r subtries equal to

$$\mathcal{T}(\boldsymbol{x}_{\langle 0 \rangle}), \ldots, \mathcal{T}(\boldsymbol{x}_{\langle r-1 \rangle}),$$

where $\boldsymbol{x}_{\langle \sigma \rangle}$ denotes the sequence consisting of words of $\boldsymbol{x}$ which begin with symbol σ, stripped of their initial symbol σ. If the set $\boldsymbol{x}_{\langle \sigma \rangle}$ is non-empty, the edge which links the subtrie $\mathcal{T}(\boldsymbol{x}_{\langle \sigma \rangle})$ to the internal node is labelled with the symbol σ.

x_1	`cacccaaac...`
x_2	`aaacacbac...`
x_3	`aaabcbbca...`
x_4	`bacbaabcc...`
x_5	`bcabbbbbc...`
x_6	`bacaabbba ...`
x_7	`ccbacbcbb...`



In this paper, we perform a probabilistic analysis of the shape of $\mathcal{T}(\boldsymbol{x})$. In our probabilistic model, the sequence $\boldsymbol{x}$ is formed with words that are independently drawn from the source $\mathcal{S}$, and we are interested in the asymptotics when the cardinality n of $\boldsymbol{x}$ tends to ∞. Here, we focus on a particular parameter of the trie, called the depth, and denoted by D_n: it is defined as the depth D_n of a *random* branch, and it is now described.

Given a sequence $\boldsymbol{x} = (x_1, \ldots, x_n)$, the trie $\mathcal{T}(\boldsymbol{x})$ has exactly n branches, and the length (or the depth) of a branch is the number of the nodes it contains. For $i \in [1..n]$, the length of the i–th branch of the trie (corresponding to the word x_i) is denoted by $D_n^{(i)}$. Inside our model, the depth D_n of a random branch satisfies

$$\Pr[D_n \geq k+1] = \frac{1}{n} \sum_{i=1}^{n} \Pr[D_n^{(i)} \geq k+1]. \tag{7}$$

The parameter D_n will be simply called the trie depth. For a fixed source, this is a random variable which depends on the set $\boldsymbol{x}$ of words emitted by the source, and the (well-known) next proposition studies its moments. We remark that Assertion (iii) is less classical.

▶ **Proposition 7.** *Consider a probabilistic source and a set of n infinite words independently emitted by the source. Then, the depth D_n of the trie built on this set satisfies the following:*

(i) *The distribution of D_n involves the fundamental probabilities of the source,*

$$\Pr[D_n \geq k+1] = \sum_{|w|=k} p_w[1-(1-p_w)^{n-1}] = \frac{1}{n} \sum_{|w|=k} \sum_{\ell=2}^{n} (-1)^\ell \binom{n}{\ell} \ell\, p_w^\ell \qquad \textit{for } k \geq 0.$$

(ii) *If the generating series $\Lambda(s)$ is well-defined for $s \geq 2$, then the expectation $\mathbb{E}[D_n]$ is expressed as an alternating sum which involves the values $\Lambda(\ell)$, for $\ell \geq 2$*

$$\mathbb{E}[D_n] = \frac{1}{n} \sum_{\ell=2}^{n} (-1)^\ell \binom{n}{\ell} \ell\, \Lambda(\ell). \tag{8}$$

(iii) *As soon as the source contains, for each $k \geq 1$, a prefix of length $k-1$ whose probability is at least Ak^{-a} with $a \leq 1$ for some $A > 0$, all the moments of D_n of order k for any $n \geq 2$ and $k \geq 2$ are infinite.*

Proof.

(i) The event $D_n^{(i)} \geq k+1$ means that there exists a prefix w of length k that is common to the word x_i and at least to another word x_j of the sequence. Inside our model, this entails the first expression in (i), and, with a binomial expansion, the second one.

(ii) Now, if $\Lambda(2)$ is finite, any $\Lambda(\ell)$ is also finite for $\ell \geq 2$. Taking the sum over k of the previous expression entails (ii), after the exchange of two summations (over k and over n).

(iii) The sequence $n \mapsto \Pr[D_n \geq k]$ is increasing, and it is thus sufficient to deal with the case $n = 2$. Under the assumption, one has

$$\Pr[D_2 \geq k] = \sum_{|w|=k-1} p_w^2 \geq A^2\, k^{-2a}\,,$$

$$\begin{aligned}\mathbb{E}[D_2^2] &= \sum_{k\geq 1} k^2 \Big(\Pr[D_2 \geq k] - \Pr[D_2 \geq k+1] \Big) \\ &= \sum_{k\geq 1} (2k-1)\Pr[D_2 \geq k] \geq A^2 \sum_{k\geq 1} k^{1-2a}\,.\end{aligned}$$

All the moments $\mathbb{E}[D_n^k]$ are thus infinite for $n \geq 2, k \geq 2$ as soon as $a \leq 1$. ◀

▶ **Proposition 8.** *For the two sources, the moments $\mathbb{E}[D_n^k]$ of order $k \geq 2$ are infinite.*

Proof. For each source, the prefix 0^k has a probability $1/(k+1)$. Then (iii) applies. ◀

3.2 Survey for the Rice method

The rest of the paper then studies the mean value $\mathbb{E}[D_n]$, starting with its expression given in (8). We will use here the Rice method, that is dedicated to the study of sequences $n \mapsto f(n)$ that are expressed as a binomial sum which involves another sequence $n \mapsto p(n)$,

$$f(n) = \sum_{\ell=a}^{n} (-1)^\ell \binom{n}{\ell} p(\ell)\,, \qquad (a \text{ integer}, a \geq 0; \text{ here } a = 2). \tag{9}$$

The method was introduced by Nörlund [17, 18] and widely used in analytic combinatorics since the seminal papers of Flajolet and Sedgewick [9, 8]. See also the survey in [24]. The main role is then played by the analytical extension ψ of the sequence $n \mapsto p(n)$, provided it be *tame at $s = c$* for $c < a$. We now recall this notion:

▶ **Definition 9.** *A function $\psi(s)$ is tame at c with order d if there exists $\delta_0 > 0$, called the tameness width, for which*

(i) *$\psi(s)$ is analytic on $\Re s > c - \delta_0$ except at $s = c$ where it admits a pole of order $d > 0$, with a singular expression at $s = c$ of the form $\psi(s) \asymp a_d(s-c)^{-d} + \ldots + a_1(s-c)^{-1} + a_0$.*

(ii) *For any $\delta < \delta_0$, $\psi(s)$ is of polynomial growth on $\Re s \geq c - \delta$ as $|\Im s| \to \infty$.*

There are three main steps in the method.

Step 1. The inequality $c < a$ entails that ψ is analytic on $\Re s > a$, and the binomial formula is transfered into a Rice integral formula.

Consider a real c with $c \in]a-1, a[$. Then, for any $b \in]c, a[$ and $n \geq n_0$, the sequence $f(n)$ admits an integral representation

$$f(n) = \sum_{\ell=a}^{n} (-1)^\ell \binom{n}{\ell} p(\ell) = \frac{1}{2i\pi} \int_{b-i\infty}^{b+i\infty} L_n(s)\cdot\psi(s)\, ds\,, \qquad L_n(s) := \frac{\Gamma(n+1)\Gamma(-s)}{\Gamma(n+1-s)}\,.$$

Step 2. This integral representation is valid for any abscissa $b \in]c, a[$. The vertical line $\Re s = b$ is shifted to the left, using the tameness properties of ψ on the left,

For any $\delta < \delta_0$, the following asymptotic formula involving the tameness width δ holds:

$$f(n) = \text{Res}\,[L_n(s) \cdot \psi(s); s = c] + O(n^{c-\delta}), \quad (n \to \infty)\,.$$

Step 3. The residue $\text{Res}\,[L_n(s) \cdot \psi(s); s = c]$ admits the estimate

$$A_n[\psi] := \text{Res}\,[L_n(s) \cdot \psi(s); s = c] = n^c \cdot P(\log n)\,[1 + O(1/n)]\,, \tag{10}$$

and involves a polynomial P that is computed from the singular expansion of $\psi(s)$ and $\Gamma(-s)$ at $s = c$, with two cases:

(i) If c is integer, $\Gamma(-s)$ has also a pole at $s = c$, and the product $\Gamma(-s) \cdot \psi(s)$ has a pole of order $d + 1$. Then the polynomial P has degree d, with a dominant term equal to $[1/\Gamma(d + 1)]\,|a_d|$. We remark that the factor $[1 + O(1/n)]$ equals 1 in the case $c = 1$.

(ii) If c is not an integer, the product $\Gamma(-s) \cdot \psi(s)$ has a pole of order d, and $P(t)$ has degree $d - 1$, with a dominant term equal to $[\Gamma(-c)/\Gamma(d)]\,|a_d|$.

4 Tameness of the generating functions. Main result

We thus study the function $s \mapsto s\Lambda(s)$ for each source. We wish to prove that it is tame at $s = c$ with $c > 2$ and some order d. We have to make precise the location of the dominant pole $s = c$, its order, and prove the polynomial growth of $s\Lambda(s)$ on a half-plane $\Re s > c - \delta$. We then compute the residue $A_n[s\Lambda(s)]$ defined in (10) following the principles of the previous Step 3. Remembering the division by n in Eq. (8), we finally obtain our main result.

4.1 The Stern-Brocot source

The iterate $\mathbf{A}_s^n$ of the operator $\mathbf{A}_s$ is written as

$$\mathbf{A}_s^n[F](x, y) = \left| \left(\frac{1}{1 + nx} \right) \left(\frac{1}{1 + ny} \right) \right|^s F\left(\frac{x}{1 + nx}, \frac{y}{1 + ny} \right)\,.$$

Then, in particular, when $(x, y) = (0, 1)$, the quasi-inverse writes as

$$(I - \mathbf{A}_s)^{-1}[L](0, 1) = L(0, 1) + \sum_{n \geq 1} \left(\frac{1}{n + 1} \right)^s L\left(0, \frac{1}{n + 1}\right)\,. \tag{11}$$

With Proposition 3, this is applied to the DGF $\Lambda(s)$,

$$\Lambda(s) = L_s(0, 1) + \sum_{n \geq 1} \left(\frac{1}{n + 1} \right)^s L_s\left(0, \frac{1}{n + 1}\right), \qquad \text{with} \quad L_s := (I - \mathbf{G}_s)^{-1}[1]\,. \tag{12}$$

As L_s belongs to $\mathcal{C}^1([0, 1]^2)$ (see Proposition 10), one deals with $M_s : y \mapsto (\partial/\partial y)L_s(0, y)$, and the following estimate holds:

$$\Lambda(s) = \zeta(s)L_s(0, 0) + O\left(\zeta(s + 1)\right) ||M_s||_0\,, \qquad ||F||_0 := \sup\{|F(x, y)| \mid (x, y) \in [0, 1]^2\}\,. \tag{13}$$

We now use deep results due to Dolgopyat in [6], that have been adapted by Baladi and Vallée in [1] to the plain quasi-inverse $(I - G_s)^{-1}$, then extended by Cesaratto and Vallée [4] to the quasi-inverse of the secant operator $\mathbf{G}_s$. They prove the following:

▶ **Proposition 10** (Dolgopyat, Baladi, Cesaratto, Vallée). *The mapping $s \mapsto L_s := (I - \mathbf{G}_s)^{-1}[1]$ viewed as a mapping from $\mathbb{C}$ to $\mathcal{C}^1([0,1]^2)$ is analytic for $\Re s > 1-\delta$, except at $s=1$, where it has a simple pole, and is of polynomial growth in the half-plane $\Re s > 1-\delta$ for $|\Im s| \to \infty$ for some $\delta > 0$. Moreover, for s close to 1*

$$L_s(x,y) \sim_{s\to 1} \frac{1}{\mathcal{E}}\frac{1}{s-1}\Phi(x,y), \qquad M_s(x,y) := \frac{\partial}{\partial y}L_s(x,y) \sim_{s\to 1} \frac{1}{\mathcal{E}}\frac{1}{s-1}\frac{\partial}{\partial y}\Phi(x,y)\,. \quad (14)$$

Here, Φ is the extension[3] *of the Gauss density $\phi(x) = (1/\log 2)(1/(1+x))$ and satisfies $\Phi(0,0) = \phi(0) = 1/(\log 2)$ and $\mathcal{E}$ is the entropy of the Gauss map, equal to $(1/\log 2)\zeta(2)$.*

The expression (12) and the estimate (13) prove that $\Lambda(s)$ is analytic for $\Re s > 1$. Then, with (12) and (14), we see that $s = 1$ is a pole of order 2 for $\Lambda(s)$, with the estimate

$$\Lambda(s) \sim_{s\to 1} \zeta(s)\left[\frac{1}{\mathcal{E}}\frac{1}{s-1}\Phi(0,0)\right] \sim_{s\to 1} \frac{1}{\zeta(2)}\left(\frac{1}{s-1}\right)^2.$$

We now study the tameness of $\Lambda(s)$ at $s=1$. The function $\zeta(s)$ is tame at $s=1$, with a tameness width equal to 1, as it will be recalled in Lemma 12. The functions L_s and M_s are tame at $s=1$, as it was recalled in Proposition 10, with a tameness width $\delta < 1$. Finally:

▶ **Proposition 11.** *The DGF $\Lambda(s)$ of the Stern-Brocot source is analytic on $\Re s > 1-\delta$ (for some $\delta > 0$), except at $s=1$, where it has a pole of order 2. It is of polynomial growth on $\Re s \geq 1-\delta$ for $|\Im s| \to \infty$. Moreover, the following estimates hold:*

$$s\Lambda(s) \sim_{s\to 1} \frac{1}{\zeta(2)}\left(\frac{1}{s-1}\right)^2 \qquad \Gamma(-s)\cdot s\Lambda(s) \sim_{s\to 1} \frac{6}{\pi^2}\left(\frac{1}{s-1}\right)^3.$$

Using then Step 3 of Section 3.2, the equality holds for the residue defined in (10)

$$A_n[s\cdot\Lambda(s)] = n\,P_2(\log n), \qquad P_2(t) = \frac{3}{\pi^2}\,t^2 + b_1\,t + b_0 \qquad \text{for some constants } b_1, b_0\,. \quad (15)$$

4.2 The Sturm source

With the expression of $\Lambda(s)$ given in (4), we need properties of the zeta functions (plain or double), together with its inverse $1/\zeta(s)$. They are recalled in the following Lemma.

▶ **Lemma 12.** *The following holds for the functions ζ and $1/\zeta$:*
(a) *For any $a_0 > 0$, the function $\zeta(s)$ is meromorphic on the half-plane $\Re s > 2a_0$ with only a simple pole at $s=1$ and is of polynomial growth on $\Re s \geq 2a$, with $a > a_0$ for $|\Im s| \to \infty$.*
(b) *For any $b_0 > 0$, the function $1/\zeta(s)$ is analytic on the half-plane $\Re s > 1+2b_0$ and its modulus is less than $\zeta(1+2b)$ on any half-plane $\Re s \geq 1+2b$ with $b > b_0$.*

Proof. Assertion (a) is classical and proven for instance in [21], Chapter II.3, Theorem 7.
Assertion (b) is a consequence of Mertens' inequality recalled in Chapter II.3, Corollary 8.1 of [21], that provides an upper bound for $1/\zeta(s)$

$$|\zeta(\sigma+i\tau)|^{-4} \leq \zeta(\sigma)^3|\zeta(\sigma+2i\tau)| \qquad \text{for } \sigma \geq 1+2b > 1,\ b > 0\,.$$

Using the inequality $|\zeta(\sigma+2i\tau)| \leq \zeta(\sigma)$, we obtain $|\zeta(\sigma+i\tau)|^{-1} \leq \zeta(\sigma) \leq \zeta(1+2b)$. ◀

[3] precisely described in [22, Théorème 5, Eq. (48)].

We now return to the double zeta function. The following estimate holds on $\Re s > 1$, and relates the double zeta function and the plain zeta function

$$\zeta(s, s-1) = \frac{1}{s-1}\zeta(2s-2) + O(\zeta(2s-1)).$$

Then, Assertion (a) of Lemma 12 shows that $\zeta(s, s-1)$ is analytic on $\Re s > 1 + a_0$ $(a_0 > 0)$ with a pole only at $s = 3/2$, and a residue equal to 1. It is of polynomial growth for $|\Im s| \to \infty$ on $\Re s \geq 1 + a$ for $a > a_0$. Furthermore, with Assertion (b) of Lemma 12, the inverse $1/\zeta(2s-1)$ is analytic on $\Re s > 1 + b_0$ $(b_0 > 0)$ and of polynomial growth on $\Re s \geq 1 + b$ for $b > b_0$. Choosing $a_0 = b_0$ provides a tameness width $\delta > 1/2 - \epsilon$ for any $\epsilon > 0$. Finally:

▶ **Proposition 13.** *For any $a_0 > 0$, the DGF $\Lambda(s)$ of the Sturm source is analytic on $\Re s > 1 + a_0$, except at $s = 3/2$ where it admits a simple pole. It is of polynomial growth on $\Re s \geq 1 + a$ for any $a > a_0$. Moreover, the following estimate holds:*

$$s\Lambda(s) \sim_{s\to 3/2} \frac{36}{\pi^2}\left(\frac{1}{2s-3}\right) \qquad \Gamma(-s)\cdot s\Lambda(s) \sim_{s\to 3/2} \frac{36}{\pi^2}\Gamma(-3/2)\left(\frac{1}{2s-3}\right).$$

Using then Step 3 of Section 3.2, and the value $\Gamma(-3/2) = (4/3)\sqrt{\pi}$, the following estimate holds for the residue defined in (10):

$$A_n[s\cdot\Lambda(s)] = \frac{24}{\pi^{3/2}} n^{3/2}\left[1 + O(1/n)\right]. \tag{16}$$

4.3 Statement of the main result

Using Step 3 of Section 3.2, with the estimates of the residue $A_n[s\Lambda(s)]$ obtained in (15) and (16), together with the remainder term associated with the tameness strip, and remembering the division by n in Eq. (8), we obtain our final result.

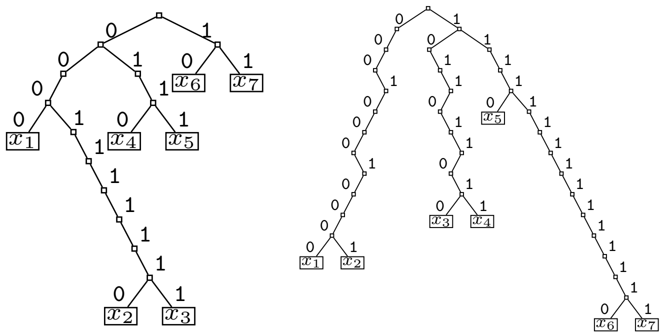


Figure 3 Instances of tries built on seven words emitted from each source of interest: the Stern-Brocot source (on the left), the Sturm Source (in the middle). As the value $n = 7$ is small, and the moments $\mathbb{E}[D_n^2]$ are infinite, there does not really exist a "typical trie". The third trie (on the right) is built on seven words emitted by the Farey dynamical source mentioned in the Conclusion.

▶ **Theorem 14.** *Consider, for each source, a trie built on n words independently drawn from the source. Then, the mean value of the trie depth grows as $\Theta(\log^2 n)$ for the Stern-Brocot source whereas it grows as $\Theta(n^{1/2})$ for the Sturm source,*

$$\text{[Stern-Brocot case]} \qquad \mathbb{E}[D_n] = \frac{3}{\pi^2}\log^2 n + b_1 \log n + b_0 \; + O(n^{-\delta}) \quad \textit{for some } \delta > 0;$$

$$\text{[Sturm case]} \qquad \mathbb{E}[D_n] = \frac{24}{\pi^{3/2}} n^{1/2} + O(n^a) \quad \textit{for any } a > 0.$$

Figure 3 clearly exhibits some important features of each source. This explains –in an experimental way– why the trie is a good tool for studying the characteristics of a source.

5 Conclusions and further work

This paper appears as (one of) the first study dedicated to sources of zero Shannon entropy, and performed with Analytic Combinatorics tools. It focuses on a particular parameter of the source, the trie depth. We wish to extend this first study in several directions.

We wish to use Analytic Combinatorics tools, notably singularity analysis, to directly derive estimates of Prop. 6, that are presently obtained via fine Number Theory arguments. It is probably possible to directly deal with the bivariate DGF $\Lambda(s, v)$, whose expression seems closely related (in both cases) to generalized versions of the polylogarithm. We then hope using the methods of Flajolet in [7], dedicated to singularity analyses of the polylogarithm. This will be a first step towards the distribution of the coincidence C_n defined in Section 2.2.

The VLMC sources (VLMC = Variable Length Markov Chain) are the simplest sources where the dependency from the past is unbounded. The paper [3] deeply studies this model and analyzes the depth of associated suffix tries in some particular cases.
We wish to focus on a whole natural sub-class of VLMC sources, related to the intermittency phenomenon. We consider the binary case, assume the equality $\Pr[Y_0 = 1] = 1$, and focus on the events $\mathcal{S}_k :=$ [the prefix finishes with a sequence of exactly k occurrences of 0].
A VLMC is *intermittent of exponent* $a > 0$ when the following conditional probability distribution holds: $\Pr[0 \mid \mathcal{S}_0] = (1/2)$, $\Pr[0 \mid \mathcal{S}_k] = (k/(k+1))^a$, $(k \geq 1)$.
Then, the series $\Lambda(s)$ involves two functions of Riemann ζ type, and strongly depends on the parameter a. We wish to perform a complete analysis of the trie depth for this precise class, exhibiting the dependence with respect to parameter a.

Fig 3 exhibits an instance of a trie built on the Farey dynamical source. As recalled in Section 2.4, the Farey DS admits the Stern-Brocot partition as a generating partition. Moreover, the Farey DS admits, as an invariant density, the density $1/t$ whose integral is infinite. Then, the fundamental probabilities of the two sources [Stern-Brocot and Farey] are not clearly related. This strongly differs from the framework of the papers [5, 11, 4] which deal with ergodic dynamical sources, whose invariant measure is absolutely continuous with respect to the Lebesgue measure. Then, the analysis of trie depth for the Farey source will be both a natural and difficult question.

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A Appendix

We now give two proofs of the fact that the Shannon entropy $\mathcal{E}$ of the Stern-Brocot source is zero.

A.1 About the entropy of the Stern-Brocot source. Analytical proof

We follow the approach of Prellberg and Slawny [19] that we adapt to our framework, and there are three steps in the proof. The first two steps deal with the case $s < 1$, and the third step lets $s \to 1$.

Step 1. We study the operator $\mathbf{G}_{s,v}$ for a pair (s,v), with s real, $s \in]1/2, 1[$ and v complex. For $|v| < 1$, this operator acts on the space $\mathcal{C}^1([0,1]^2)$. When v is real, with $0 < v < 1$, it admits a unique dominant eigenvalue denoted as $\lambda(s,v)$ that depends analytically on the pair (s,v). There is an inequality which relates the spectral radii, $r[\mathbf{G}_{s,v}] \le r[\mathbf{G}_{s,|v|}] = \lambda(s,|v|)$.

For $v \to 0$, the eigenvalue $\lambda(s,v)$ tends to 0, whereas it coincides at $v = 1$ with the dominant eigenvalue $\lambda(s)$ of $\mathbf{G}_{s,1} = \mathbf{G}_s$ that is strictly larger than 1 for $s < 1$. There thus exists, for any $s < 1$, a real number $v = v(s)$ for which the operator $\mathbf{G}_{s,v(s)}$ has a dominant eigenvalue $\lambda(s, v(s))$ equal to 1.

Moreover, for any pair (v_1, v_2), with $v_1 < v_2$, the inequality $\lambda(s,v_2) \ge \lambda(s,v_1)\,[v_2/v_1]$ holds, and entails the following:

(i) for any $v < v(s)$, the strict inequality $\lambda(s,v) < 1$

(ii) the inequality $\lambda'_v(s, v(s)) > 0$.

The Implicit Function Theorem can be applied, and it defines a real analytic function $v :]1/2, 1[\to]0, 1[$ that satisfies the equation

$$\lambda'_s(s, v(s)) + v'(s)\lambda'_v(s, v(s)) = 0\,. \tag{17}$$

All these remarks entail, that, for any $s \in]1/2, 1[$, there exists $w(s) > v(s)$ for which the quasi-inverse $v \mapsto (I - \mathbf{G}_{s,v})^{-1}[1]$ is meromorphic for $|v| < w(s)$ with only a (simple) pole at $v = v(s)$, with the estimate,

$$(I - \mathbf{G}_{s,v})^{-1}[1] \sim_{v \to v(s)} \frac{\lambda(s, v(s))}{1 - \lambda(s, v(s))} \Psi_{s,v} e_{s,v(s)}[1]\,,$$

so that the residue at $v = v(s)$ is

$$a(s) = \frac{1}{\lambda'_v(s, v(s))} \Psi_{s,v(s)}\, e_{s,v(s)}[1] \tag{18}$$

and defines an analytical map $s \mapsto a(s)$ for $s \in]1/2, 1[$.

Step 2. We return to the operator $\mathbf{H}_s$ (and its quasi-inverse). For any $\Psi \in \mathcal{C}^1([0,1]^2)$, the mapping $v \mapsto (I - v\mathbf{A}_s)^{-1}[\Psi](0,1)$ is well defined and analytic for $v < 1$. Then, with Proposition 3, the previous properties can be transfered to the quasi-inverse $v \mapsto (I - v\mathbf{H}_s)^{-1}[1](0,1)$: it is meromorphic for $v < u(s) := \min(1, w(s))$ with a unique pole (simple) at $v = v(s)$, and we remark the strict inequality $u(s) > v(s)$ for $s \in]1/2, 1[$. Then, with singularity analysis of meromorphic functions, [for instance Theorem IV.10 p. 258 in [10]], we obtain

$$\mathbf{H}_s^k[1](0,1) = v(s)^{-k} \cdot a(s) \left[1 + O\left(\frac{u(s)}{v(s)}\right)^{-k} \right], \qquad \text{for } k \to \infty\,,$$

where the coefficient $a(s)$ is related to dominant spectral properties of $\mathbf{G}_{s,v(s)}$ and is strictly positive (see (18)). Now, the analytical dependence with respect to s entails that, on any closed interval $[s_0, s_1]$ with $1/2 < s_0 < s_1 < 1$, the ratio $v(s)/u(s)$ is bounded by a constant $b < 1$, whereas $|a(s)|$ and $|v'(s)|$ admit strictly positive lower bounds and $s \mapsto |a'(s)|$ an upper bound. One has there

$$e_k(s) := \sum_{|w|=k} p_w^s = \mathbf{H}_s^k[1](0,1) = v(s)^{-k} \cdot a(s) \left[1 + O(b^k)\right] \qquad \text{for } k \to \infty\,.$$

One then takes the derivative with respect to s,

$$\frac{1}{k}e_k'(s) = \frac{1}{k}\sum_{|w|=k} p_w^s \log p_w = -v'(s)\, v(s)^{-k-1}\, a(s)\, \left[1+\frac{1}{k}\frac{a'(s)}{a(s)}\frac{v(s)}{v'(s)}\right] [1+O(b^k)]$$

$$= -v'(s)\, v(s)^{-k-1}\, a(s)\, \left[1+O\left(\frac{1}{k}\right)\right] \qquad \text{for } k\to\infty\,.$$

As this is true on any interval $[s_0, s_1] \subset]1/2, 1[$, we deduce the asymptotic behaviour for any $s \in]1/2, 1[$,

$$\lim_{k\to\infty}\frac{1}{k}\left[\frac{e_k'(s)}{e_k(s)}\right] = -\frac{v'(s)}{v(s)}\,. \tag{19}$$

Step 3. When $s \to 1$. Due to the equality $\mathbf{G}_{s,1} = \mathbf{G}_s$, the operator $\mathbf{G}_{s,1}$ has a dominant eigenvalue equal to 1, and the function $s \mapsto v(s)$ may be extended at $s = 1$ via the equality $\lim_{s\to 1^-} v(s) = v(1) = 1$. Moreover, as $s \to 1^-$, the derivative $\lambda_s'(s, v(s))$ has a limit (equal to the derivative of the dominant eigenvalue $\lambda'(s)$ at $s = 1$), and thus the second term in (17) has also a limit: as we have already seen, the derivative $\lambda_v'(s, 1)$ is closely related to $\zeta(2s-1)$ and tends to ∞ for $s \to 1$, and this entails that $\lim_{s\to 1^-} v'(s) = 0$. Finally the right member of (19) has a limit when $s \to 1^-$, and thus

$$\lim_{s\to 1}\lim_{k\to\infty}\frac{1}{k}\left[\frac{e_k'(s)}{e_k(s)}\right] = 0\,.$$

We are interested in the following limit (if it exists)

$$\lim_{k\to\infty}\frac{1}{k}\left[\frac{e_k'(1)}{e_k(1)}\right] = \lim_{k\to\infty}\frac{1}{k}\lim_{s\to 1}\left[\frac{e_k'(s)}{e_k(s)}\right]\,,$$

and we thus wish to exchange the limits. This is possible if we have uniform convergence of the derivatives. Uniform convergence holds in the context of monotonic functions whose (simple) limit is continuous. Here, this is the case: as the functions $s \mapsto e_k(s)$ are log concave for any k, thus, for any k, the quotient $s \mapsto e_k'(s)/e_k(s)$ defines a decreasing mapping of s, whereas the map $s \mapsto v'(s)/v(s)$ is continuous on $]1/2, 1[$ and extended with its limit when $s \to 1^-$. This legitimates the exchange of limits, and

$$\lim_{k\to\infty}\frac{1}{k}\left[\frac{e_k'(1)}{e_k(1)}\right] = \lim_{s\to 1}\lim_{k\to\infty}\frac{1}{k}\left[\frac{e_k'(s)}{e_k(s)}\right] = 0\,.$$

A.2 About the entropy of the Stern-Brocot source. Ergodic proof

Step 1. Two sources and their fundamental intervals. Both sources, the Stern-Brocot source and the Farey source, are associated with the binary coding, corresponding to the choice of the inverse branches

$$a\colon x \mapsto \frac{x}{1+x}, \quad \text{when } x < 1/2, \qquad b\colon x \mapsto \frac{1}{1+x}, \quad \text{when } x > 1/2.$$

Any Farey fundamental interval J_w is associated with a binary word $w \in \{a, b\}^\star$. Due to the equality $\{a, b\}^\star = \{a^\star b\}^\star \cdot a^\star$, any binary word $w \in \{a, b\}^k$ is written in a unique way as

$$[a^{n_1} b]\cdot[a^{n_2} b]\cdot\ldots\cdot[a^{n_\ell} b]\cdot a^r, \qquad \ell + r + \sum_{j=1}^{\ell} n_j = k, \quad r \ge 0, \quad n_j \ge 0\ \ (\forall j \in [1, \ell])\,. \tag{20}$$

The integer m_j defined for $j \in [1 \dots \ell]$ as $m_j := n_j + 1$ satisfies $m_j \geq 1$, and the Farey LFT $a^{m-1} \circ b$ coincides with the `Cfe` LFT $g_m : x \mapsto 1/(m+x)$. Third, the LFT a^r is of the form $a^r : x \mapsto x/(1+rx)$. Then, the Farey LFT h_w associated with the word w is related to the sequence $\boldsymbol{m} = (m_1, m_2, \dots, m_\ell)$ via the `Cfe` LFT $g_{\boldsymbol{m}} := g_{m_1} \circ g_{m_2} \dots \circ g_{m_\ell}$ and the relation $h_w = g_{\boldsymbol{m}} \circ a^r$ holds.
Finally, the Farey fundamental interval $J_w = [h_w(0), h_w(1)]$ associated with the word w coincides with the interval $[g_m(0), g_m(1/(1+r))]$. Then its length p_w involves r together the coefficients of the LFT $g_m(x) := (ax+b)/(cx+d)$. The equality $|ad - bc| = 1$ holds; moreover the denominator coefficients satisfy $0 \leq c \leq d$, and the coefficient d coincides with the continuant $q(\boldsymbol{m})$ relative to the sequence $\boldsymbol{m} = (m_1, m_2, \dots m_\ell)$. Then, one has

$$p_w = \left| g_{\boldsymbol{m}}(0) - g_{\boldsymbol{m}}\left(\frac{1}{1+r}\right) \right| = \frac{1}{d(c + d(1+r))} \geq \frac{1}{d^2(r+2)}\,, \qquad \frac{1}{p_w} \leq q(\boldsymbol{m})^2 (r+2)\,. \tag{21}$$

Step 2. Changing base. For $\boldsymbol{m} \in \mathbb{N}^\star$, we denote by $\ell(\boldsymbol{m})$ the number of components of $\boldsymbol{m}$, by $c(\boldsymbol{m})$ the sum of the components of $\boldsymbol{m}$, by $q(\boldsymbol{m})$ the continuant associated with $\boldsymbol{m}$. We now fix a length k (that will tend to ∞ later). With $x \in [0,1]$, we associate the word $w_{\langle k \rangle}(x)$ of length k produced by the Stern-Brocot source on x. With (20), it defines almost everywhere a pair $(\boldsymbol{m}(x), r(x))$ with $\boldsymbol{m}(x) \in \mathbb{N}^\star$ and $r(x) \geq 0$, that depends on x and the depth k. It is thus denoted as $(\boldsymbol{m}_{\langle k \rangle}(x), r_{\langle k \rangle}(x))$ and the equality $c(\boldsymbol{m}_{\langle k \rangle}(x)) + r_{\langle k \rangle}(x) = k$ holds. It is clear (but important) to remark the following: as x belongs to the `Cfe` interval relative to $\boldsymbol{m}_{\langle k \rangle}(x)$, then the sequence $\boldsymbol{m}_{\langle k \rangle}(x)$ provides the beginning of the `Cfe` of x. Of course, this production may be quite slow (when $\ell_{\langle k \rangle}(x)$ is much smaller than k), and this is why the entropy of the Stern-Brocot source will be zero.
We then define three random variables on the unit interval that depend on k and relate the `Cfe` of x together its Farey expansion of depth k,

$$\ell\langle k \rangle(x) := \ell(\boldsymbol{m}_{\langle k \rangle}(x)), \quad c_{\langle k \rangle}(x) := c(\boldsymbol{m}_{\langle k \rangle}(x)) = m_1(x) + \ldots + m_{\ell_{\langle k \rangle}(x)}(x), \tag{22}$$

$$q_{\langle k \rangle}(x) := q(\boldsymbol{m}_{\langle k \rangle}(x)) = q(m_1(x), \dots, m_{\ell_{\langle k \rangle}(x)}(x))\,. \tag{23}$$

By definition of the process, for each k, the inequality $\boldsymbol{\ell}_{\langle k \rangle}(x) \leq \boldsymbol{c}_{\langle k \rangle}(x) \leq k$ holds.

Step 3. Entropy of the Stern-Brocot source. Denote by $\pi_{\langle k \rangle}(x)$ the measure of the fundamental Farey interval of depth k the input x belongs to. Then, the entropy of the Stern-Brocot source is the limit (if it exists) of the sequence $e(k)$,

$$e(k) = \frac{1}{k}\mathbb{E}\Big[|\log \pi_{\langle k \rangle}(x)|\Big] = \frac{1}{k} \sum_{w \in \{a,b\}^k} p_w \cdot |\log p_w|\,.$$

Using (21), and applying it to the pair $(\boldsymbol{m}_{\langle k \rangle}(x), r_{\langle k \rangle}(x))$, one obtains

$$\frac{1}{\pi_{\langle k \rangle}(x)} \leq q_{\langle k \rangle}(x)^2 \cdot (r_{\langle k \rangle}(x) + 2)\,; \qquad |\log \pi_{\langle k \rangle}(x)| \leq 2 \log q_{\langle k \rangle}(x) + \log(r_{\langle k \rangle}(x) + 2)\,. \tag{24}$$

As the bound $r_{\langle k \rangle}(x) \leq k$ holds, this entails the inequality

$$e(k) \leq \frac{1}{k}\log(k+2) + 2d(k), \qquad d(k) = \mathbb{E}\left[\frac{1}{k}\log q_{\langle k \rangle}(x)\right]. \tag{25}$$

As the first term in (25) tends to 0 for $k \to \infty$, we then focus on the second term $d(k)$.

We first remark that the sequence $k \mapsto \ell_{\langle k \rangle}(x)$ is increasing (not strictly in general). Then, there are two cases: it is bounded (and then stationary) or it tends to ∞. For an input x, the sequence $\ell_{\langle k \rangle}(x)$ is stationary if and only if the Farey word produced on x finishes by an infinite sequence of a or by a b. This arises if and only if x is rational. Then, almost everywhere, the increasing sequence $k \mapsto \ell_{\langle k \rangle}(x)$ tends to ∞.

Step 4. Application of the Dominated Convergence Theorem. We now show that the sequence $d(k)$ tends to 0 with the Dominated Convergence Theorem. We thus use two inequalities for the random variable $f_k(x) := (1/k) \log q_{\langle k \rangle}(x)$. One has always, for any $m \in \mathbb{N}^\star$,

$$q(\boldsymbol{m}) \le \prod_{i=1}^{\ell(m)} (m_i + 1) \qquad \text{and} \qquad \log q(\boldsymbol{m}) \le \sum_{i=1}^{\ell(m)} \log(m_i+1) \le \sum_{i=1}^{\ell(m)} m_i = c(\boldsymbol{m})\,. \quad (26)$$

Applied to $\boldsymbol{m} := \boldsymbol{m}_{\langle k \rangle}(x)$, this proves the domination :

$$\frac{1}{k} \log q_{\langle k \rangle}(x) \le \frac{c_{\langle k \rangle}(x)}{k} \le 1 \qquad \text{for almost every } x \in [0,1] \ .$$

Moreover, for any $\boldsymbol{m} \in \mathbb{N}^\star$, using again (26) in a more precise way, we derive the bound

$$\frac{1}{k} \log q(\boldsymbol{m}) \le \left[\frac{c(\boldsymbol{m})}{k}\right] \left[\frac{\ell(\boldsymbol{m})}{c(\boldsymbol{m})}\right] \left[\frac{1}{\ell(\boldsymbol{m})} \sum_{i=1}^{\ell(m)} \log(m_i+1)\right] ,$$

that holds in particular for $\boldsymbol{m} = \boldsymbol{m}_{\langle k \rangle}(x)$.

The first factor is now at most 1 for $x \in [0,1]$. Furthermore, almost everywhere, the sequence $\ell_{\langle k \rangle}(x) \to \infty$ when $k \to \infty$. Then, with the Ergodic Theorem, the third factor tends almost everywhere to a finite limit C. Furthermore, using a result due to Khinchin described in [15, Theorem 35], together the Ergodic Theorem applied to the sequence $\min(M, m_i)$ (for any given constant M), the second factor also tends to 0 almost everywhere. Finally, the sequence $x \mapsto (1/k) \log q_{\langle k \rangle}(x)$ tends almost everywhere to 0.

We now apply the dominated convergence theorem to the sequence of random variables $f_k(x) = (1/k) \log q_{\langle k \rangle}(x)$ that is bounded by 1 and converges to 0 almost everywhere. This proves that $d(k)$ tends to 0. This is the same for the initial entropy sequence $e(k)$.

The k-Cut Model in Conditioned Galton-Watson Trees

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Abstract

The k-cut number of rooted graphs was introduced by Cai et al. [7] as a generalization of the classical cutting model by Meir and Moon [16]. In this paper, we show that all moments of the k-cut number of conditioned Galton-Watson trees converge after proper rescaling, which implies convergence in distribution to the same limit law regardless of the offspring distribution of the trees. This extends the result of Janson [13].

2012 ACM Subject Classification Mathematics of computing → Probabilistic algorithms

Keywords and phrases k-cut, cutting, conditioned Galton-Watson trees

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.5

Related Version A full version of the paper is available at [4], `http://arxiv.org/abs/1907.02770`.

Funding This work is supported by the Knut and Alice Wallenberg Foundation, the Swedish Research Council and The Swedish Foundations' starting grant from Ragnar Söderbergs Foundation.

1 Introduction and main result

In order to measure the difficulty for the destruction of a resilient network Cai et al. [7] introduced a generalization of the cut model of Meir and Moon [16] where each vertex (or edge) needs to be cut $k \in \mathbb{N}$ times (instead of only once) before it is destroyed. More precisely, consider that the resilient network is a rooted tree $\mathbb{T}_n$, with $n \in \mathbb{N}$ vertices. We destroy it by removing its vertices as follows: **Step 1:** Choose a vertex uniformly at random from the component that contains the root and cut the selected vertex once. **Step 2:** If this vertex has been cut k times, remove the vertex together with the edges attached to it from the tree. **Step 3:** If the root has been removed, then stop. Otherwise, go to step **Step 1**. We let $\mathcal{K}_k(\mathbb{T}_n)$ denote the (random) total number of cuts needed to end this procedure the k-cut number, i.e., $\mathcal{K}_k(\mathbb{T}_n)$ models how much effort it takes to destroy the network. (For simplicity, we will omit the subscript k and write $\mathcal{K}(\mathbb{T}_n)$.) It should be plain that one can define analogously an edge deletion version of the previous algorithm, where one needs to cut an edge k times before removing it from the root component. Then, one would be interested in the number $\mathcal{K}_e(\mathbb{T}_n)$ of cuts needed to isolate the root of $\mathbb{T}_n$.

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31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 5; pp. 5:1–5:10
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

The case $k = 1$ (i.e., the traditional cutting model of Meir and Moon [16]) has been well-studied by several authors in the past few decades. More precisely, Meir and Moon estimated the first and second moment of the 1-cut number in the cases when $\mathbb{T}_n$ is a Cayley tree [16] and a recursive tree [17]. Subsequently, several weak limit theorems for the 1-cut number have been obtained for Cayley trees (Panholzer [18, 19]), complete binary trees (Janson [12]), conditioned Galton-Watson trees (Janson [13] and Addario-Berry et al. [1]), recursive trees (Drmota et al. [8], Iksanov and Möhle [11]), binary search trees (Holmgren [9]) and split trees (Holmgren [10]). In the general case $k \geq 1$, the authors in [7] established first moment estimates of $\mathcal{K}(\mathbb{T}_n)$ for families of deterministic and random trees, such as paths, complete binary trees, split trees, random recursive trees and conditioned Galton-Watson trees. In particular, the authors in [7] have proven a weak limit theorem for $\mathcal{K}(\mathbb{T}_n)$ when $\mathbb{T}_n$ is a path consisting of n vertices. More recently, Cai and Holmgren [6] obtained also a weak limit theorem in the case when $\mathbb{T}_n$ is a complete binary tree.

In this work, we continue the investigation of this general cutting-down procedure in conditioned Galton-Watson trees and show that $\mathcal{K}(\mathbb{T}_n)$, after a proper rescaling, converges in distribution to a non-degenerate random variable. More precisely, let ξ be a non-negative integer-valued random variable such that

$$\mathbb{E}[\xi] = 1 \quad \text{and} \quad 0 < \sigma^2 \coloneqq \mathrm{Var}(\xi) < \infty, \tag{1}$$

and consider a Galton-Watson process with (critical) offspring distribution ξ. Let $\mathbb{T}_n$ be the family tree conditioned on its number of vertices being $n \in \mathbb{N}$. The main result of this paper is the following. We write $\xrightarrow{d}$ to denote convergence in distribution. (In the rest of the paper CRT stands for Continuum Random Tree.)

▶ **Theorem 1.** *Let $k \in \mathbb{N}$. Let $\mathbb{T}_n$ be a Galton-Watson tree conditioned on its number of vertices being $n \in \mathbb{N}$ with offspring distribution ξ satisfying* (1)*. Then,*

$$\sigma^{-1/k} n^{-1+1/2k} \mathcal{K}(\mathbb{T}_n) \xrightarrow{d} Z_{\mathrm{CRT}}, \quad \text{as } n \to \infty, \tag{2}$$

where Z_{CRT} is a non-degenerate random variable whose law is determined entirely by its moments: $\mathbb{E}[Z^0_{\mathrm{CRT}}] = 1$, and for $q \in \mathbb{N}$, $\mathbb{E}[Z^q_{\mathrm{CRT}}] = \eta_{k,q}$ with

$$\eta_{k,q} \coloneqq q! \int_0^\infty \cdots \int_0^\infty y_1(y_1 + y_2) \cdots (y_1 + \cdots + y_q) e^{-\frac{(y_1 + \cdots + y_q)^2}{2}} F_q(\boldsymbol{y}_q) \, \mathrm{d}y_q \cdots \mathrm{d}y_1, \tag{3}$$

where $\boldsymbol{y}_q = (y_1, \ldots, y_q) \in \mathbb{R}^q_+$ and

$$F_q(\boldsymbol{y}_q) \coloneqq \int_0^\infty \int_0^{x_1} \cdots \int_0^{x_{q-1}} \exp\left(-\frac{y_1 x_1^k + y_2 x_2^k + \cdots + y_q x_q^k}{k!} \right) \mathrm{d}x_q \cdots \mathrm{d}x_2 \, \mathrm{d}x_1.$$

Furthermore, if $\mathbb{E}[\xi^p] < \infty$ for every $p \in \mathbb{Z}_{\geq 0}$, then for every $q \in \mathbb{Z}_{\geq 0}$,

$$\sigma^{-q/k} n^{-q+q/2k} \mathbb{E}[\mathcal{K}(\mathbb{T}_n)^q] \to \mathbb{E}[Z^q_{\mathrm{CRT}}]$$

as $n \to \infty$.

In the case $k = 1$, Theorem 1 reduces to Z_{CRT} having a Rayleigh distribution with density $xe^{-x^2/2}$, for $x \in \mathbb{R}_+$. More precisely, one can verify that $\eta_{1,q} = 2^{q/2}\Gamma(1 + q/2)$, for $q \in \mathbb{Z}_{\geq 0}$, which are the moments of a random variable with the Rayleigh distribution; in this paper $\Gamma(\cdot)$ denotes the well-known gamma function. As we mentioned early, the case $k = 1$ has been shown in [13, Theorem 1.6] (or Addario-Berry et al. [1]). We henceforth assume throughout this paper that $k \geq 2$. It is also important to mention that we could not find a simpler expression (in general) for the moments $\eta_{k,q}$ except for some particular instances. For $q = 1$, we have

$$\eta_{k,1} = 2^{-\frac{1}{2k}} \frac{(k!)^{\frac{1}{k}}}{k} \Gamma\left(\frac{1}{k}\right) \Gamma\left(1 - \frac{1}{2k}\right).$$

Then Theorem 1 provides a proof of [7, Lemma 4.10], where an estimation for the first moment of $\mathcal{K}(\mathbb{T}_n)$ was first announced but whose proof was left to the reader, see Lemma 10. On the other hand, let $(U_1, \dots, U_q)$ be q i.i.d. leaves of a Brownian CRT and define the vector $(L_0^{\text{CRT}}, L_1^{\text{CRT}}, \dots, L_q^{\text{CRT}})$ where $L_0^{\text{CRT}} = 0$ and L_i^{CRT} is the total length of a Brownian CRT reduced to the leaves of $U_1, \dots, U_i$; see [3, Lemma 21] from where one can deduce explicitly the distribution of $(L_0^{\text{CRT}}, L_1^{\text{CRT}}, \dots L_q^{\text{CRT}})$. From the proof of Theorem 1, we obtain, for $q \in \mathbb{N}$, that

$$\eta_{k,q} = q! \int_0^\infty \int_0^{x_1} \cdots \int_0^{x_{q-1}} \mathbb{E}\left[\exp\left(-\frac{\sum_{i=1}^q (L_i^{\text{CRT}} - L_{i-1}^{\text{CRT}}) x_i^k}{k!}\right)\right] \mathrm{d}\bar{\mathbf{x}}_q,$$

where $\bar{\mathbf{x}}_q = (x_q, \dots, x_1) \in \mathbb{R}_+^q$. This suggests that it ought to be possible to build the random variable Z_{CRT} by some construction that can be interpreted as the k-cut model on the Brownian CRT defined by Aldous [2, 3]. The appearance of the Brownian CRT in this framework should not come as a surprise since it is well-known that if we assign length $n^{-1/2}$ to each edge of the Galton-Watson tree $\mathbb{T}_n$, then the latter converges weakly to a Brownian CRT as $n \to \infty$.

The approach used in this work consists of implementing an extension of the idea of Janson [13], which was used in [7], in order to study the k-cut model on deterministic and random trees. The authors in [7] introduced an equivalent model that allows them to define $\mathcal{K}(\mathbb{T}_n)$ in terms of the number of records in $\mathbb{T}_n$ when vertices are assigned random labels. More precisely, let $(E_{i,v})_{i \geq 1, v \in \mathbb{T}_n}$ be a sequence of independent exponential random variables of parameter 1; Exp(1) for short. Let $G_{r,v} \coloneqq \sum_{1 \leq i \leq r} E_{i,v}$, for $r \in \mathbb{N}$ and $v \in \mathbb{T}_n$. Clearly, $G_{r,v}$ has a gamma distribution with parameters $(r, 1)$, which we denote by Gamma(r). Imagine that each vertex $v \in \mathbb{T}_n$ has an alarm clock and v's clock fires at times $(G_{r,v})_{r \geq 1}$. If we cut a vertex when its alarm clock fires, then due to the memoryless property of exponential random variables, we are actually choosing a vertex uniformly at random to cut. However, this also means that we are cutting vertices that have already been removed from the tree. Thus, for a cut on vertex v at time $G_{r,v}$ (for some $r \in \{1, \dots, k\}$) to be counted in $\mathcal{K}(\mathbb{T}_n)$, none of its strict ancestors can already have been cut k times, i.e.,

$$G_{r,v} < \min\{G_{k,u} : u \in \mathbb{T}_n \text{ and } u \text{ is a strict ancestor of } v\}.$$

When the previous event happens, we say that $G_{r,v}$, or simply v, is an r-record and let

$$I_{r,v} \coloneqq [\![G_{r,v} < \min\{G_{k,u} : u \in \mathbb{T}_n \text{ and } u \text{ is a strict ancestor of } v\}]\!], \tag{4}$$

where $[\![\cdot]\!]$ denotes the Iverson bracket, i.e., $[\![S]\!] = 1$ if the statement S is true and $[\![S]\!] = 0$ otherwise. Let $\mathcal{K}_r(\mathbb{T}_n)$ be the number of r-records, i.e., $\mathcal{K}_r(\mathbb{T}_n) \coloneqq \sum_{v \in \mathbb{T}_n} I_{r,v}$. Then, it should be plain that

$$\mathcal{K}(\mathbb{T}_n) \stackrel{d}{=} \sum_{1 \leq r \leq k} \mathcal{K}_r(\mathbb{T}_n), \tag{5}$$

where $\stackrel{d}{=}$ denotes equal in distribution.

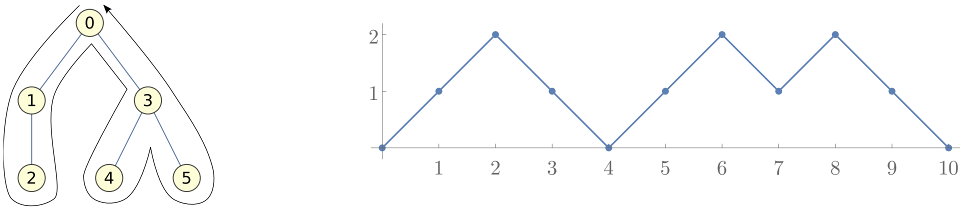

Figure 1 An example of a depth-first walk in a tree and the corresponding V_n.

Loosely speaking, we then consider the well-known *depth-first* walk $(V_n(t), t \in [0, 2(n-1)])$ of the tree $\mathbb{T}_n$ as depicted in Figure 1, that is, $V_n(t)$ is "the depth of the t-th vertex" visited in this walk; this will be made precise in the next section. As it is well-known (see Aldous [3, Theorem 23 with Remark 2] or [15, Theorem 1]), when T_n is a conditioned Galton-Watson with offspring distribution satisfying (1), we have that

$$(n^{-1/2}V_n(2(n-1)t), t \in [0,1]) \xrightarrow{d} 2\sigma^{-1}B^{\text{ex}}, \qquad \text{as } n \to \infty.$$

in $C([0,1], \mathbb{R}_+)$, with its usual topology, and where $B^{\text{ex}} = (B^{\text{ex}}(t), t \geq 0)$ is a standard normalized Brownian excursion. It has been shown in [7, Lemma 1] that $\mathbb{E}[I_{r,v}] \sim C_{r,k} d_n(v)^{-r/k}$, for some (explicit) constant $C_{r,k} > 0$, where $d_n(v)$ is the depth of the vertex $v \in \mathbb{T}_n$. Let $\circ$ denote the root of $\mathbb{T}_n$. Thus, informally

$$\begin{aligned}
&\mathbb{E}\left[\mathcal{K}_r(\mathbb{T}_n) \mid \mathbb{T}_n\right] \\
&\sim \sum_{v \in \mathbb{T}_n \setminus \{\circ\}} \frac{C_{r,k}}{d_n(v)^{r/k}} \sim \frac{C_{r,k}}{2} \int_0^{2(n-1)} \frac{\mathrm{d}t}{V_n(t)^{r/k}} \sim \frac{C_{r,k}}{n^{-1+\frac{r}{2k}}} \int_0^1 \left(\frac{V_n(2(n-1)t)}{\sqrt{n}}\right)^{-\frac{r}{k}} \mathrm{d}t \\
&\sim \frac{C_{r,k}}{n^{-1+\frac{r}{2k}}} \left(\frac{\sigma}{2}\right)^{\frac{r}{k}} \int_0^1 \frac{\mathrm{d}t}{B^{\text{ex}}(t)^{r/k}},
\end{aligned}$$

as $n \to \infty$. By taking expectation, we deduce that

$$\sigma^{-r/k} n^{-1+\frac{r}{2k}} \mathbb{E}\left[\mathcal{K}_r(\mathbb{T}_n)\right] \sim C_{r,k} \mathbb{E}\left[\int_0^1 (2B^{\text{ex}}(t))^{-r/k} \, \mathrm{d}t\right], \qquad \text{as } n \to \infty,$$

which coincides with the right-hand side of (3) when $r = q = 1$. Notice that this informal computation suggests that $\mathbb{E}\left[\mathcal{K}_r(\mathbb{T}_n)\right] = O(n^{1-\frac{r}{2k}})$, for $r \in \{1, \ldots, k\}$. As a consequence, the Markov's inequality implies $n^{-1+\frac{1}{2k}} \mathcal{K}_r(\mathbb{T}_n) \to 0$ in probability, as $n \to \infty$, for $r \in \{2, \ldots, k\}$. If so, by the identity in (5), it would be enough to prove Theorem 1 for $\mathcal{K}_1(\mathbb{T}_n)$ instead of $\mathcal{K}(\mathbb{T}_n)$.

In the rest of the paper, we make the above argument precise and extend it to higher moments in order to apply the method of moments for proving Theorem 1. In a full version of this paper [4], we also apply the same idea to get all moments of the number of records in paths and several types of trees of logarithmic height, e.g., complete binary trees, split trees, uniform random recursive trees and scale-free trees. We omit the proofs of our more technical lemmas since they can be found in [4].

2 Preliminary results

The purpose of this section is to establish a general convergence result for the number of 1-records $\mathcal{K}_1(\mathbb{T}_n)$ of a deterministic rooted ordered tree $\mathbb{T}_n$. The results of this section can also be viewed as a generalization of those of Janson [13] and Cai, et al. [7]. Furthermore, these results will allow us to study the convergence of the cut number $\mathcal{K}(\mathbb{T}_n)$ not only for conditioned Galton-Watson trees in Section 3, but also for other classes of random trees in a full version of this paper [4].

We start by defining a probability measure through a continuous function in the same spirit as in [13, Theorem 1.9]. Let $I \subseteq \mathbb{R}_+$ be an interval. For a function $f : I \to \mathbb{R}_+$ and $t_1, \dots, t_q \in I$ with $q \in \mathbb{N}$, we define

$$L_f(t_1, \dots, t_q) \coloneqq \sum_{i=1}^{q} f(t_{(i)}) - \sum_{i=1}^{q-1} \inf_{t \in [t_{(i)}, t_{(i+1)}]} f(t), \tag{6}$$

where $t_{(1)}, \dots, t_{(q)}$ are $t_1, \dots, t_q$ arranged in nondecreasing order. Notice that $L_f(t_1, \dots, t_q)$ is symmetric in $t_1, \dots, t_q$ and that $L_f(t) = f(t)$ for $t \in I$. Define

$$D_f(t_1) \coloneqq L_f(t_1), \qquad D_f(t_1, \dots, t_q) \coloneqq L_f(t_1, \dots, t_q) - L_f(t_1, \dots, t_{q-1}), \quad \text{for} \quad q \geq 2. \tag{7}$$

We also consider the functional

$$G_f(\mathbf{t}_q, \mathbf{x}_q) \coloneqq \exp\left(-\frac{D_f(t_1)x_1^k + \cdots + D_f(t_1, \dots, t_q)x_q^k}{k!} \right), \tag{8}$$

for $\mathbf{x}_q = (x_1, \dots, x_q) \in \mathbb{R}_+^q$ and $\mathbf{t}_q = (t_1, \dots, t_q) \in I^q$. If $I = [0, 1]$, we further define, for $q \in \mathbb{N}$, let $m_0(f) \coloneqq 1$ and

$$m_q(f) \coloneqq q! \int_0^1 \int_0^1 \cdots \int_0^1 \int_0^\infty \int_0^{x_1} \cdots \int_0^{x_{q-1}} G_f(\mathbf{t}_q, \mathbf{x}_q)\, \mathrm{d}\overleftarrow{\mathbf{x}}_q\, \mathrm{d}\overleftarrow{\mathbf{t}}_q, \quad q \geq 2, \tag{9}$$

where $\overleftarrow{\mathbf{x}}_q = (x_q, \dots, x_1)$ and $\overleftarrow{\mathbf{t}}_q = (t_q, \dots, t_1)$.

▶ **Theorem 2.** *Let $k \in \mathbb{N}$. Suppose that $f \in C([0,1], \mathbb{R}_+)$ is such that $\int_0^1 f(t)^{-1/k} \mathrm{d}t < \infty$. Then there exists a unique probability measure ν_f on $[0, \infty)$ with finite moments given by*

$$\int_{[0,\infty)} x^q \nu_f(\mathrm{d}x) = m_q(f), \qquad \textit{for} \ \ q \in \mathbb{Z}_{\geq 0}.$$

Consider a rooted ordered tree $\mathbb{T}_n$ with root $\circ$ and $n \in \mathbb{N}$ vertices. We now explain how $\mathbb{T}_n$ can be coded by a continuous function. We define the so-called *depth-first search function* [2, page 260], $\psi_n : \{0, 1, \dots, 2(n-1)\} \to \{\text{vertices of } \mathbb{T}_n\}$ such that $\psi_n(i)$ is the $(i+1)$-th vertex visited in a depth-first walk on the tree starting from the root $\circ$. Note that $\psi_n(i)$ and $\psi_n(i+1)$ always are neighbours, and thus, we extend ψ to $[0, 2(n-1)]$ by letting, for $1 \leq i < t < i+1 \leq 2(n-1)$, $\psi_n(t)$ to be the one of $\psi_n(i)$ and $\psi_n(i+1)$ that has largest depth (recall that the depth of a vertex $v \in \mathbb{T}_n$ is the distance, i.e., number of edges, between $\circ$ to v). Let $d_n(v)$ be the depth of a vertex $v \in \mathbb{T}_n$. We further define the *depth-first walk* V_n of $\mathbb{T}_n$ by

$$V_n(i) \coloneqq d_n(\psi(i)), \qquad 0 \leq i \leq 2(n-1),$$

and extend V_n to $[0, 2(n-1)]$ by linear interpolation. Thus $V_n \in C([0, 2(n-1)], \mathbb{R}_+)$. See Figure 1 for an example of V_n. Furthermore, we normalize the domain of V_n to $[0, 1]$ by defining

$$\widetilde{V}_n(t) \coloneqq V_n(2(n-1)t) \quad \text{and} \quad \widehat{V}_n(t) \coloneqq \lceil V_n(2(n-1)t) \rceil, \tag{10}$$

for $t \in [0, 1]$. Thus $\widetilde{V}_n, \widehat{V}_n \in C([0,1], \mathbb{R}_+)$. Note that $d_n(\psi(t)) = \lceil V_n(t) \rceil$, for $t \in [0, 2(n-1)]$. Moreover,

$$\max_{v \in \mathbb{T}_n} d_n(v) = \sup_{t \in [0, 2(n-1)]} V_n(t) = \sup_{t \in [0,1]} \widetilde{V}_n(t). \tag{11}$$

We now state the central result of this section, that is, a general limit theorem in distribution for the number of 1-records $\mathcal{K}_1(\mathbb{T}_n)$ of a deterministic rooted tree $\mathbb{T}_n$ with n vertices. It is important to notice that $\mathcal{K}_1(\mathbb{T}_n)$ is a random variable since the 1-records are random.

▶ **Lemma 3.** *Let $k \in \mathbb{N}$. Suppose that $(\mathbb{T}_n)_{n\geq 1}$ is a sequence of (deterministic) ordered rooted trees, and denote the corresponding normalized depth-first walks by $\widetilde{V}_n$ and $\widehat{V}_n$. Suppose that there exists a sequence $(a_n)_{n\geq 1}$ of non-negative real numbers with $\lim_{n\to\infty} a_n = 0$, $\lim_{n\to\infty} na_n^{1/k} = \infty$ and a function $f \in C([0,1], \mathbb{R}_+)$ such that*
(a) *$a_n\widetilde{V}_n(t) \to f(t)$, in $C([0,1], \mathbb{R}_+)$, as $n \to \infty$.*
(b) *$\int_0^1 (a_n\widehat{V}_n(t))^{-1/k}\,\mathrm{d}t \to \int_0^1 f(t)^{-1/k}\,\mathrm{d}t < \infty$, as $n \to \infty$.*
Then, for each $q \in \mathbb{Z}_{\geq 0}$,

$$n^{-q}a_n^{-q/k}\mathbb{E}[\mathcal{K}_1(\mathbb{T}_n)^q] \to m_q(f),$$

as $n \to \infty$, where $m_q(f)$ is defined in (9). Moreover, $n^{-1}a_n^{-1/k}\mathcal{K}_1(\mathbb{T}_n) \xrightarrow{d} Z_f$, as $n \to \infty$, where Z_f is a random variable with distribution ν_f defined by Theorem 2.

We can apply similar ideas as in the proofs of Lemma 3 in order to estimate the mean of the number of r-records $\mathcal{K}_r(\mathbb{T}_n)$. It is important to mention that we have not tried to estimate higher moments of $\mathcal{K}_r(\mathbb{T}_n)$ in order to obtain a limit theorem in distribution for this quantity. We believe that our methods can be used but the computations will be more involved and we decided not to do it. Furthermore, the next results shows that $\mathcal{K}_r(\mathbb{T}_n)$ is of smaller order than $\mathcal{K}_1(\mathbb{T}_n)$ and hence it will not contribute (in the limit) to the distribution of the k-cut number $\mathcal{K}(\mathbb{T}_n)$.

▶ **Lemma 4.** *Let $k \in \mathbb{N}$. Let $\mathbb{T}_n$ be a (deterministic) rooted tree with $n \in \mathbb{N}$ vertices. Suppose that there exists a sequence $(a_n)_{n\geq 1}$ of non-negative real numbers with $\lim_{n\to\infty} a_n = 0$, $\lim_{n\to\infty} na_n = \infty$ and $\max_{v\in\mathbb{T}_n} d_n(v) = O(a_n^{-1})$. Then, for $r \in \{1, \dots, k\}$, and uniformly over $\mathbb{T}_n$,*

$$n^{-1}a_n^{-r/k}\mathbb{E}[\mathcal{K}_r(\mathbb{T}_n)] = (1 + O(a_n^{\frac{1}{2k}}))\int_0^1\int_0^\infty \frac{x^{r-1}e^{-a_n^{1/k}x}}{\Gamma(r)}e^{-\frac{a_n\widehat{V}_n(t)x^k}{k!}}\,\mathrm{d}x + o(1).$$

▶ **Lemma 5.** *Let $k \in \mathbb{N}$. Suppose that $(\mathbb{T}_n)_{n\geq 1}$ is a sequence of (deterministic) ordered rooted trees. Suppose that there exists a sequence $(a_n)_{n\geq 1}$ of non-negative real numbers with $\lim_{n\to\infty} a_n = 0$, $\lim_{n\to\infty} na_n = \infty$ and a function $f \in C([0,1], \mathbb{R}_+)$ such that $\widetilde{V}_n$ satisfies the condition (a) in Lemma 3 and that for $r \in \{1, \dots, k\}$,*

$$\int_0^1 (a_n\widehat{V}_n(t))^{-r/k}\,\mathrm{d}t \to \int_0^1 f(t)^{-r/k}\,\mathrm{d}t < \infty, \quad \text{as } n \to \infty.$$

Then,

$$n^{-1}a_n^{-r/k}\mathbb{E}[\mathcal{K}_r(\mathbb{T}_n)] \to \frac{(k!)^{r/k}\Gamma(r/k)}{k\Gamma(r)}\int_0^1 f(t)^{-r/k}\,\mathrm{d}t, \quad \text{as } n \to \infty.$$

3 Proof of Theorem 1

Let $\mathbb{T}_n$ be a Galton-Watson tree conditioned on its number of vertices being $n \in \mathbb{N}$ with offspring distribution ξ satisfying (1). Notice that in this case both the r-records and the tree are random. Then we study $\mathcal{K}_r(\mathbb{T}_n)$ as random variable conditioned on $\mathbb{T}_n$. More precisely, we first choose a random tree $\mathbb{T}_n$. Then we keep it fixed and consider the number of r-records. This gives a random variable $\mathcal{K}_r(\mathbb{T}_n)$ with distribution that depends on $\mathbb{T}_n$. We have the following lemma that corresponds to [13, Lemma 4.8].

▶ **Lemma 6.** *Let $k \in \mathbb{N}$. Let $\mathbb{T}_n$ be a Galton-Watson tree conditioned on its number of vertices being $n \in \mathbb{N}$ with offspring distribution ξ satisfying (1). For $r \in \{1, \ldots, k\}$. We have that $\mathbb{E}[\mathcal{K}_r(\mathbb{T}_n)] = O(n^{1-\frac{r}{2k}})$.*

Proof. By an application of Lemma 4 with $a_n = n^{-1/2}$, we see that

$$\begin{aligned}
\mathbb{E}[\mathcal{K}_r(\mathbb{T}_n)|\mathbb{T}_n] &\leq (1 + O(a_n^{\frac{1}{2k}})) \sum_{v \in \mathbb{T}_n \setminus \{\circ\}} \int_0^\infty \frac{x^{r-1}}{\Gamma(r)} e^{-\frac{d_n(v) x^k}{k!}} \, \mathrm{d}x + o(n a_n^{r/k}) \\
&= (1 + O(a_n^{\frac{1}{2k}})) \sum_{v \in \mathbb{T}_n \setminus \{\circ\}} \frac{(k!)^{r/k} \Gamma(r/k)}{k \Gamma(r)} d_n(v)^{-r/k} + o(n a_n^{r/k}) \\
&= (1 + O(a_n^{\frac{1}{2k}})) \frac{(k!)^{r/k} \Gamma(r/k)}{k \Gamma(r)} \sum_{i=1}^\infty i^{-r/k} w_i(\mathbb{T}_n) + o(n a_n^{r/k}),
\end{aligned} \tag{12}$$

where $w_i(\mathbb{T}_n)$ denotes the number of vertices at depth $i \in \mathbb{N}$ in $\mathbb{T}_n$. Notice that

$$\sum_{i=1}^\infty i^{-r/k} w_i(\mathbb{T}_n) \leq n^{1-\frac{r}{2k}} + \sum_{i=1}^{\lfloor n^{1/2} \rfloor} i^{-r/k} w_i(\mathbb{T}_n),$$

by the fact that $\sum_{i \geq 0} w_i(\mathbb{T}_n) = n$. Since $\mathbb{E}[\xi^2] < \infty$ by our assumption (1), [13, Theorem 1.13] implies that for all $n, i \in \mathbb{N}$, $\mathbb{E}[w_i(\mathbb{T}_n)] \leq Ci$ for some constant $C > 0$ depending on ξ only. Therefore,

$$\sum_{i=1}^\infty i^{-r/k} \mathbb{E}[w_i(\mathbb{T}_n)] = n^{1-\frac{r}{2k}} + \sum_{i=1}^{\lfloor n^{1/2} \rfloor} \mathbb{E}[w_i(\mathbb{T}_n)] i^{-\frac{1}{k}} = O(n^{1-\frac{r}{2k}}). \tag{13}$$

By taking expectation in (12), our claim follows by (13). ◀

We continue by studying the moments of the number of 1-records $\mathcal{K}_1(\mathbb{T}_n)$. We denote by μ_n the (random) probability distribution of $\sigma^{-1/k} n^{-1+1/2k} \mathcal{K}_1(\mathbb{T}_n)$ given $\mathbb{T}_n$. Define the random variables

$$m_q(\mathbb{T}_n) := \mathbb{E}[\mathcal{K}_1(\mathbb{T}_n)^q | \mathbb{T}_n], \qquad q \in \mathbb{Z}_{\geq 0}.$$

Notice that the moments of μ_n are given by $\sigma^{-q/k} n^{-q+q/2k} m_q(\mathbb{T}_n)$. We have the following lemma that corresponds to [13, Lemma 4.9].

▶ **Lemma 7.** *Let $k \in \mathbb{N}$. Let $\mathbb{T}_n$ be a Galton-Watson tree conditioned on its number of vertices being $n \in \mathbb{N}$ with offspring distribution ξ satisfying* (1)*. Furthermore, suppose that for every fixed $q \in \mathbb{N}$ we have that $\mathbb{E}[\xi^{q+1}] < \infty$. Then $\mathbb{E}[m_q(\mathbb{T}_n)] = O(n^{q-\frac{q}{2k}})$.*

Let $\widetilde{V}_n$ and $\widehat{V}_n$ be the normalized depth-first walks associated with the conditioned Galton-Watson tree $\mathbb{T}_n$. Notice that in this case $\widetilde{V}_n$ and $\widehat{V}_n$ become random functions on $C([0,1], \mathbb{R}_+)$. Recall that a remarkable result due to Aldous [3, Theorem 23 with Remark 2] (see also [15, Theorem 1]) shows that

$$n^{-1/2} \widetilde{V}_n \xrightarrow{d} 2\sigma^{-1} B^{\text{ex}}, \qquad \text{as } n \to \infty, \tag{14}$$

in $C([0,1], \mathbb{R}_+)$, with its usual topology, and where $B^{\text{ex}} = (B^{\text{ex}}(t), t \geq 0)$ is a standard normalized Brownian excursion. Notice that B^{ex} is a random element in $C([0,1], \mathbb{R}_+)$; see for example [5] or [20].

▶ **Lemma 8.** *Let $k \in \mathbb{N}$. For $r \in \{1, \ldots, k\}$, we have that $\int_0^1 B^{\mathrm{ex}}(t)^{-r/k}\,\mathrm{d}t < \infty$ almost surely.*

Proof. One only needs to show that $\mathbb{E}[\int_0^1 B^{\mathrm{ex}}(t)^{-r/k}\,\mathrm{d}t] < \infty$. This follows by computing $\mathbb{E}[B^{\mathrm{ex}}(t)^{-r/k}]$, for every $t \in [0,1]$, from the well-known density function of $B^{\mathrm{ex}}(t)$; see [5, Chapter II, Equation (1.4)]. ◀

Therefore, Theorem 2 and Lemma 8 imply that there exists almost surely a (unique) measure $\nu_{2B^{\mathrm{ex}}}$ with moments given by $m_q(2B^{\mathrm{ex}})$. The next result provides a generalization of [13, Theorem 1.10] and it will be used in the proof of Theorem 1.

▶ **Theorem 9.** *Let $k \in \mathbb{N}$. Let $\mathbb{T}_n$ be a Galton-Watson tree conditioned on its number of vertices being $n \in \mathbb{N}$ with offspring distribution ξ satisfying* (1)*. Then*

$$\mu_n \xrightarrow{d} \nu_{2B^{\mathrm{ex}}}, \qquad \text{as } n \to \infty, \tag{15}$$

in the space of probability measures on $\mathbb{R}$. Moreover, we have that for every $q \in \mathbb{N}$,

$$\sigma^{-q/k} n^{-q+q/2k} m_q(\mathbb{T}_n) \xrightarrow{d} m_q(2B^{\mathrm{ex}}), \qquad \text{as } n \to \infty. \tag{16}$$

The convergences in (14)*,* (15) *and* (16)*, for all $q \in \mathbb{N}$, hold jointly. In particular, if $\mathbb{E}[\xi^p] < \infty$ for all $p \in \mathbb{N}$, then for all $q \in \mathbb{N}$ and $l \in \mathbb{N}$,*

$$\sigma^{-lq/k} n^{-lq/k+lq/2k} \mathbb{E}[m_q(\mathbb{T}_n)^l] \to \mathbb{E}[m_q(2B^{\mathrm{ex}})^l], \qquad \text{as } n \to \infty. \tag{17}$$

Proof. A simple adaptation of the proof for [13, Lemma 4.7] easily shows that

$$\left(\widetilde{V}_n, \int_0^1 \widehat{V}_n(t)^{-1/k}\,\mathrm{d}t\right) \xrightarrow{d} \left(2\sigma^{-1}B^{\mathrm{ex}}, 2^{-1/k}\sigma^{1/k}\int_0^1 B^{\mathrm{ex}}(t)^{-1/k}\,\mathrm{d}t\right), \quad \text{in } C([0,1], \mathbb{R}_+), \tag{18}$$

as $n \to \infty$. By the Skorohod coupling theorem (see e.g. [14, Theorem 4.30]), we can assume that the trees $(\mathbb{T}_n)_{n\geq 1}$ are defined on a common probability space such that the convergence in (18) holds almost surely. Therefore, the convergences (15) and (16) follow immediately from Lemma 3. It only remains to prove (17). Recall that we assume that $\mathbb{E}[\xi^p] < \infty$ for every $p \in \mathbb{N}$. By Jensen's inequality, we notice that $m_q(\mathbb{T}_n)^l \leq m_{lq}(\mathbb{T}_n)$ for $l, q \in \mathbb{N}$. Hence Lemma 7 implies that $\mathbb{E}[m_q(\mathbb{T}_n)^l] = O(n^{lq - \frac{lq}{2k}})$. This shows that every moment of the right-hand side of (16) stays bounded as $n \to \infty$ which implies (17). ◀

Proof of Theorem 1. Lemma 6 establishes that $\mathbf{E}[\mathcal{K}_r(\mathbb{T}_n)] = O(n^{1-\frac{r}{2k}})$ for $r \in \{1, \ldots, k\}$. As a consequence, the Markov's inequality implies $n^{-1+\frac{1}{2k}}\mathcal{K}_r(\mathbb{T}_n) \to 0$ in probability, as $n \to \infty$, for $r \in \{2, \ldots, k\}$. Then, by the identity in (5), it is enough to prove Theorem 1 for $\mathcal{K}_1(\mathbb{T}_n)$ instead of $\mathcal{K}(\mathbb{T}_n)$. By the definition of μ_n and Theorem 9, for any bounded continuous function $g : \mathbb{R}_+ \to \mathbb{R}_+$,

$$\mathbb{E}[g(\sigma^{-1/k} n^{-1+1/2k} \mathcal{K}_1(\mathbb{T}_n)) | \mathbb{T}_n] = \int g\,\mathrm{d}\mu_n \xrightarrow{d} \int g\,\mathrm{d}\nu_{2B^{\mathrm{ex}}}, \qquad \text{as } n \to \infty.$$

Taking expectations, the dominated convergence theorem implies that

$$\sigma^{-1/k} n^{-1+1/2k} \mathcal{K}_1(\mathbb{T}_n) \xrightarrow{d} Z_{\mathrm{CRT}},$$

as $n \to \infty$, where Z_{CRT} has distribution $\nu(\cdot) = \mathbb{E}[\nu_{2B^{\mathrm{ex}}}(\cdot)]$. Suppose that $\mathbb{E}[\xi^p] < \infty$ for every $p \in \mathbb{N}$. Lemma 7 implies that every moment of $n^{-1+1/2k}\mathcal{K}_1(\mathbb{T}_n)$ stays bounded as $n \to \infty$ which implies the moment convergence in Theorem 1. It remains to identify the moments of Z_{CRT} (or equivalently ν). Notice that

$$\mathbb{E}[Z_{\mathrm{CRT}}^q] = \int x^q \, \mathrm{d}\nu = \mathbb{E}\left[\int x^q \, \mathrm{d}\nu_{2B^{\mathrm{ex}}}\right] = \mathbb{E}[m_q(2B^{\mathrm{ex}})], \qquad \text{for } q \in \mathbb{N}.$$

For $q \in \mathbb{N}$, let $U_1, \ldots, U_q$ be independent random variables with the uniform distribution on $[0,1]$. Let $Y_1, \ldots, Y_q$ be the first q points in a Poisson process on $(0, \infty)$ with intensity $x\,\mathrm{d}x$, i.e., $Y_1, \ldots, Y_q$ have joint density function $y_1 \cdots y_q e^{-y_q^2/2}$ on $0 < y_1 < \cdots < y_q < \infty$. It is well-known that $L_{2B^{\mathrm{ex}}}(U_1, \ldots, U_q) \overset{d}{=} Y_q$, see, e.g., [13, Proof of Lemma 5.1]. Defining the function

$$H_{f,q}(\mathbf{t}_q) := \int_0^\infty \int_0^{x_1} \cdots \int_0^{x_{q-1}} G_f(\mathbf{t}_q, \mathbf{x}_q) \, \mathrm{d}\bar{\mathbf{x}}_q, \tag{19}$$

we see that

$$\mathbb{E}[m_q(2B^{\mathrm{ex}})] = q!\mathbb{E}[H_{2B^{\mathrm{ex}},q}(\mathbf{U}_q)] = q! \int_0^{y_1} \cdots \int_0^{y_{q-1}} \int_0^\infty y_1 \cdots y_q e^{-y_q^2/2} \widetilde{F}_q(\mathbf{y}_q) \, \mathrm{d}\mathbf{y}_q, \tag{20}$$

where $\mathbf{U}_q = (U_1, \ldots, U_q)$, $\mathbf{y}_q = (y_1, \ldots, y_q) \in \mathbb{R}_+^q$ and

$$\widetilde{F}_q(\mathbf{y}_q) := \int_0^\infty \int_0^{x_1} \cdots \int_0^{x_{q-1}} \exp\left(-\frac{y_1 x_1^k + (y_2 - y_1)x_1^k + \cdots + (y_q - y_{q-1})x_q^k}{k!}\right) \mathrm{d}\bar{\mathbf{x}}_q.$$

Finally, the expression for the moments in Theorem 1 follows by first changing the order of integration in (20) and then by making the change of variables $w_i = y_i - y_{i-1}$ for $2 \le i \le q$. ◀

Following the idea of the proof of Theorem 1, we obtain the following convergence of the first moment of the number of r-records $\mathcal{K}_r(\mathbb{T}_n)$. This provides a proof of [7, Lemma 4.10].

▶ **Lemma 10.** *Let $k \in \mathbb{N}$. Let $\mathbb{T}_n$ be a Galton-Watson tree conditioned on its number of vertices being $n \in \mathbb{N}$ with offspring distribution ξ satisfying (1). For $r \in \{1, \ldots k\}$, we have that*

$$n^{-1+\frac{r}{2k}} \mathbb{E}[\mathcal{K}_r(\mathbb{T}_n)] \to \frac{(k!)^{\frac{r}{k}}}{k} \frac{\Gamma(\frac{r}{k})\Gamma\left(1 - \frac{r}{2k}\right)}{\Gamma(r)} \left(\frac{\sigma}{\sqrt{2}}\right)^{\frac{r}{k}}, \quad \text{as } n \to \infty.$$

Proof. The proof follows by a simple adaptation of the argument used in the proof of Theorem 1 by using Lemma 5 (with $a_n = n^{-1/2}$), Lemma 6 and Lemma 8. One only needs to notice that

$$\mathbb{E}\left[\int_0^1 B^{\mathrm{ex}}(t)^{-r/k} \, \mathrm{d}t\right] = 2^{\frac{r}{2k}} \Gamma\left(1 - \frac{r}{2k}\right)$$

which follows from the well-known density function of $B^{\mathrm{ex}}(t)$; see [5, II.1.4]. ◀

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Largest Clusters for Supercritical Percolation on Split Trees

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Abstract

We consider the model of random trees introduced by Devroye [13], the so-called random split trees. The model encompasses many important randomized algorithms and data structures. We then perform supercritical Bernoulli bond-percolation on those trees and obtain a precise weak limit theorem for the sizes of the largest clusters. The approach we develop may be useful for studying percolation on other classes of trees with logarithmic height, for instance, we have also studied the case of complete d-regular trees.

2012 ACM Subject Classification Mathematics of computing → Probabilistic algorithms

Keywords and phrases Split trees, random trees, supercritical bond-percolation, cluster size, Poisson measures

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.6

Funding This work is supported by the Knut and Alice Wallenberg Foundation, the Swedish Research Council and The Swedish Foundations' starting grant from Ragnar Söderbergs Foundation.

1 Introduction

In this extended abstract, we investigate the asymptotic behaviour of the sizes of the largest clusters created by performing Bernoulli bond-percolation on random split trees. Split trees were first introduced by Devroye [13] to encompass many families of trees that are frequently used to model efficient data structures or sorting algorithms (we will be more precise shortly). Some important examples of split trees are binary search trees [18], m-ary search trees [25], quad trees [16], median-of-$(2k+1)$ trees [27], fringe-balanced trees [12], digital search trees [11] and random simplex trees [13, Example 5].

To be more precise, we consider trees T_n of large but finite size $n \in \mathbb{N}$ and perform Bernoulli bond-percolation with parameter $p_n \in [0,1]$ that depends on the size of the tree (i.e., one removes each edge in T_n with probability $1-p_n$, independently of the other edges, inducing a partition of the set of vertices into connected clusters). In particular, we are going to be interested in the supercritical regime, in the sense that with high probability, there exists a giant cluster, that is of a size comparable to that of the entire tree.

Bertoin [2] established a simple characterization of tree families with n vertices and percolation regimes which results in giant clusters. Roughly speaking, Bertoin [2] showed that the supercritical regime corresponds to percolation parameters of the form $1-p_n = c/\ell(n) + o(1/\ell(n))$ as $n \to \infty$, where $c > 0$ is fixed and $\ell(n)$ is an approximation of the height of a typical vertex in the tree structure[1]. Then the size Γ_n of the cluster containing the root satisfies $\lim_{n\to\infty} n^{-1}\Gamma_n = \Gamma(c)$ in distribution to some random variable $\Gamma(c) \not\equiv 0$. In several examples the supercritical percolation parameter satisfies

$$p_n = 1 - c/\ln n + o\left(1/\ln n\right), \tag{1}$$

for some fixed parameter $c > 0$. For example, this happens for some important families of random trees with logarithmic height, such as random recursive trees, preferential attachment trees, binary search trees; see [14], [15, Section 4.4]. In those cases the random variable $\Gamma(c)$ is an (explicit) constant and the giant cluster is unique.

A natural problem in this setting is then to estimate the size of the next largest clusters. Concerning trees with logarithmic height, Bertoin [3] proved that in the supercritical regime, the sizes of the next largest clusters of a uniform random recursive tree, normalized by a factor $\ln n/n$, converge to the atoms of some Poisson random measure; see also [1]. This result was extended by Bertoin and Bravo [4] to preferential attachment trees. A different example is the uniform Cayley trees where $\ell(n) = \sqrt{n}$ and $\Gamma(c)$ is not constant. But unlike the previous examples, the number of giant components is unbounded as $n \to \infty$; see [24, 23].

As a motivation, it is important to point out that supercritical Bernoulli bond-percolation on large but finite connected graphs is an ongoing subject of research in statistical physics and mathematics. Furthermore, the estimation of the size of the next largest clusters is a relevant question in this setting. An important example where the graph is not a tree is the case of a complete graph with n vertices. A famous result due to Erdös and Rényi (see [9]) shows that Bernoulli bond-percolation with parameter $p_n = c/n + o(1/n)$ for $c > 1$ fixed, produces with high probability as $n \to \infty$, a unique giant cluster of size close to $\theta(c)n$, where $\theta(c)$ is the unique solution to the equation $x + e^{-cx} = 1$, while the second, third, etc. largest clusters have only size of order $\ln n$.

The main purpose of this work is to investigate the case of random split trees which belong to the family of random trees with logarithmic heights; see Devroye [13]. Informally speaking, a random split tree T_n^{sp} of "size" (or cardinality) n is constructed by first distributing n balls (or keys) among the vertices of an infinite b-ary tree ($b \in \mathbb{N}$) and then removing all sub-trees without balls. Each vertex in the infinite b-ary tree is given a random non-negative split vector $\mathcal{V} = (V_1, \dots, V_b)$ such that $\sum_{i=1}^{b} V_i = 1$ and $V_i \geq 0$, are drawn independently from the same distribution. These vectors affect how balls are distributed. Its exact definition is somewhat lengthy and we postpone it to Section 1.1. An important peculiarity is that the number of vertices of T_n^{sp} is often random which makes the study of split trees usually challenging.

Recently, we have shown in [7, Lemma 1 and Lemma 2] that the supercritical percolation regime in split trees of cardinality n corresponds precisely to parameters fulfilling (1). Notice that here n corresponds to the number of balls (or keys) and not to the number of vertices. More precisely, let C_n^0 (resp. $\hat{C}_n^0$) be the number of balls (resp. number of vertices) in the percolation cluster that contains the root. Then, in the regime (1) and under some mild conditions on the split tree, it holds that

$$n^{-1}C_n^0 \xrightarrow{d} e^{-c/\mu} \qquad \left(\text{resp. } n^{-1}\hat{C}_n^0 \xrightarrow{d} \alpha e^{-c/\mu}\right), \quad \text{as } n \to \infty, \tag{2}$$

where $\mu = b\mathbb{E}[-V_1 \ln V_1]$ ($\alpha > 0$ is some constant depending on the split tree) and $\xrightarrow{d}$ denotes convergence in distribution. Furthermore, the giant cluster is unique. These results agree with that of Bertoin [2] even when the number of vertices in split trees is random and the cluster sizes can be defined as either the number of balls or the number of vertices.

[1] For two sequences of real numbers $(A_n)_{n\geq 1}$ and $(B_n)_{n\geq 1}$ such that $B_n > 0$, we write $A_n = o(B_n)$ if $\lim_{n\to\infty} A_n/B_n = 0$.

Loosely speaking, our main result shows that in the supercritical regime (1) the next largest clusters of a split tree T_n^{sp} have a size of order $n/\ln n$. Moreover, we obtain a limit theorem in terms of certain Poisson random measures. A more precise statement will be given in Theorems 1 and 2 below. These results exhibit that cluster sizes, in the supercritical regime, of split-trees, uniform recursive trees and preferential attachment trees present similar asymptotic behaviour. Finally, we point out that our present approach also applies to study the size of the largest clusters for percolation on complete regular trees (see Theorem 3).

The approach developed in this work differs from that used to study the cases of uniform random recursive trees (RRT) in [3] and preferential attachment trees in [4]. The method of [3] is based on a coupling of Iksanov and Möhle [20] connecting the Meir and Moon [22] algorithm for the isolation of the root in a RRT and a certain random walk. This makes use of special properties of recursive trees (the so-called randomness preserving property, i.e., if one removes an edge from a RRT, then the two resulting subtrees, conditionally on their sizes, are independent RRT's) which fail for split-trees. The basic idea of [4] is based on the close relation of preferential attachment trees with Markovian branching processes and the dynamical incorporation of percolation as neutral mutations. The recent work of Berzunza [5] shows that one can also relate percolation on some types of split trees (but not all) with general age-dependent branching processes (or Crump-Mode-Jagers processes) with neutral mutations. However, the lack of the Markov property in those general branching processes makes the idea of [4] difficult to implement.

A common feature in these previous works, namely [3] and [4], is that, even though one addressed a static problem, one can consider a dynamical version in which edges are removed, respectively vertices inserted, one after the other in a certain order as time passes. Here we use a fairly different route and view percolation on split trees as a static problem.

We next introduce formally the family of random split trees and relevant background, which will enable us to state our main results in Section 1.2.

1.1 Random split trees

In this section, we introduce the split tree generating algorithm with parameters $b, s, s_0, s_1, \mathcal{V}$ and n introduced by Devroye [13]. Some of the parameters are the branch factor $b \in \mathbb{N}$, the vertex capacity $s \in \mathbb{N}$, and the number of balls (or cardinality) $n \in \mathbb{N}$. The additional integers s_0 and s_1 are needed to describe the ball distribution process. They satisfy the inequalities $0 < s$, $0 \leq s_0 \leq s$, $0 \leq bs_1 \leq s + 1 - s_0$. The so-called random split vector $\mathcal{V} = (V_1, \dots, V_b)$ is a random non-negative vector with $\sum_{i=1}^{b} V_i = 1$ and $V_i \geq 0$, for $i = 1, \dots, b$.

Consider an infinite rooted b-ary tree $\mathbb{T}$, i.e., every vertex has b children. We view each vertex of $\mathbb{T}$ as a bucket with capacity s and we assign to each vertex $u \in \mathbb{T}$ an independent copy $\mathcal{V}_u = (V_{u,1}, \dots, V_{u,b})$ of the random split vector $\mathcal{V}$. Let $C(u)$ denote the number of balls in vertex u, initially setting $C(u) = 0$ for all u. We call u a leaf if $C(u) > 0$ and $C(v) = 0$ for all children v of u, and internal if $C(v) > 0$ for some strict descendant v of u. The split tree T_n^{sp} is constructed recursively by distributing n balls one at time to generate a subset of vertices of $\mathbb{T}$. The balls are labeled using the set $\{1, 2, \dots, n\}$ in the order of insertion. The j-th ball is added by the following procedure.

1. Insert j to the root.
2. While j is at an internal vertex $u \in \mathbb{T}$, choose child i with probability $V_{u,i}$ and move j to child i.
3. If j is at a leaf u with $C(u) < s$, then j stays at u and $C(u)$ increases by 1.
   If j is at a leaf with $C(u) = s$, then the balls at u are distributed among u and its children as follows. We select $s_0 \leq s$ of the balls uniformly at random to stay at u. Among the

remaining $s+1-s_0$ balls, we uniformly at random distribute s_1 balls to each of the b children of u. Each of the remaining $s+1-s_0-bs_1$ balls is placed at a child vertex chosen independently at random according to the split vector assigned to u. This splitting process is repeated for any child which receives more than s balls.

We stop once all n balls have been placed in $\mathbb{T}$ and we obtain T_n^{sp} by deleting all vertices $u \in \mathbb{T}$ such that the sub-tree rooted at u contains no balls. Note that an internal vertex of T_n^{sp} contains exactly s_0 balls, while a leaf contains a random amount in $\{1, ..., s\}$. Notice also that in general the number N of vertices of T_n^{sp} is a random variable while the number of balls n is deterministic.

It is important to mention that depending on the choice of the parameters b, s, s_0, s_1 and the distribution of $\mathcal{V}$, several important data structures may be modeled. For instance, binary search trees correspond to $b = 2$, $s = s_0 = 1$, $s_1 = 0$ and $\mathcal{V}$ distributed as $(U, 1-U)$, where U is an uniform random variable on $[0, 1]$ (in this case $N = n$). Some other relevant (and more complicated) examples of split trees are m-ary search trees, median-of-$(2k + 1)$ trees, quad trees, simplex tree; see [13, 19, 10], for details and more examples.

In the present work, we assume without loss of generality that the components of the split vector $\mathcal{V}$ are identically distributed; this can be done by using random permutations as explained in [13]. In particular, we have that $\mathbb{E}[V_1] = 1/b$. We frequently use the following notation. Set

$$\mu := b\mathbb{E}[-V_1 \ln V_1]. \tag{3}$$

Note that $\mu \in (0, \ln b)$. The quantity was first introduced by Devroye [13] to study the height of T_n^{sp} as the number of balls increases.

In the study of split trees, the following condition is often assumed:

► **Condition 1.** Assume that $\mathbb{P}(V_1 = 1) = \mathbb{P}(V_1 = 0) = 0$ and that V_1 is not monoatomic, that is, $V_1 \neq 1/b$.

We sometimes consider the following condition:

► **Condition 2.** Suppose that $\ln V_1$ is non-lattice. Furthermore, for some $\alpha > 0$ and $\varepsilon > 0$,

$$\mathbb{E}[N] = \alpha n + O\left(\frac{n}{\ln^{1+\varepsilon} n}\right).$$

Recall that for two sequences of real numbers $(A_n)_{n\geq 1}$ and $(B_n)_{n\geq 1}$ such that $B_n > 0$, one writes $A_n = O(B_n)$ if $\limsup_{n\to\infty} |A_n|/B_n < \infty$. Condition 2 first appears in [10, equation (52)] for the study of the total path length of split trees.

Holmgren [19, Theorem 1.1] showed that if $\ln V_1$ is non-lattice then there exists a constant $\alpha > 0$ such that $\mathbb{E}[N] = \alpha n + o(n)$ and furthermore $Var(N) = o(n^2)$. However, this result is not enough for our purpose since an extra control in $\mathbb{E}[N]$ is needed (see Theorem 2 below). On the other hand, Condition 2 is satisfied in many interesting cases. For instance, it holds for m-ary search trees [21]. Moreover, Flajolet et al. [17] showed that for most tries (as long as $\ln V_1$ is non-lattice) Condition 2 holds. However, there are some special cases of random split trees that do not satisfy Condition 2. For instance, tries (where $s = 1$ and $s_0 = 0$) with a fixed split vector $(1/b, \ldots, 1/b)$, in which case $\ln V_1$ is lattice.

1.2 Main results

In this section, we present the main results of this work. We consider Bernoulli bond-percolation with supercritical parameter p_n satisfying (1) on T_n^{sp}. We denote by C_0 (resp. $\hat{C}_0$) the number of balls (resp. the number of vertices) of the cluster that contains the root and by $C_1 \geq C_2 \geq \cdots$ (resp. $\hat{C}_1 \geq \hat{C}_2 \geq \cdots$) the sequence of the number of balls (resp. the number of vertices) of the remaining clusters ranked in decreasing order. For the sake of simplicity, we have decided to remove the parameter n from our notation of C_i and $\hat{C}_i$.

We now state the central results of this work. The first result corresponds to the size being defined as the number of balls in the cluster.

▶ **Theorem 1.** *Let T_n^{sp} be a split tree that satisfies Condition 1 and suppose that p_n fulfills (1). Then,*

$$n^{-1} C_0 \xrightarrow{d} e^{-c/\mu}, \qquad \text{as } n \to \infty,$$

where μ is the constant defined in (3) and c is defined in (1). Furthermore, for every fixed $i \in \mathbb{N}$, we have the convergence in distribution

$$\left(\frac{\ln n}{n} C_1, \ldots, \frac{\ln n}{n} C_i \right) \xrightarrow{d} (\mathrm{x}_1, \ldots, \mathrm{x}_i), \qquad \text{as } n \to \infty,$$

where $\mathrm{x}_1 > \mathrm{x}_2 > \cdots$ denotes the sequence of the atoms of a Poisson random measure on $(0, \infty)$ with intensity $c\mu^{-1} e^{-c/\mu} x^{-2} \mathrm{d}x$.

The second result corresponds to the size being defined as the number of vertices in the cluster.

▶ **Theorem 2.** *Let T_n^{sp} be a split tree that satisfies Conditions 1-2 and suppose that p_n fulfills (1). Then,*

$$n^{-1} \hat{C}_0 \xrightarrow{d} \alpha e^{-c/\mu}, \qquad \text{as } n \to \infty,$$

where μ is the constant defined in (3), α is defined in Condition 2 and c is defined in (1). Furthermore, for every fixed $i \in \mathbb{N}$, we have the convergence in distribution

$$\left(\frac{\ln n}{n} \hat{C}_1, \ldots, \frac{\ln n}{n} \hat{C}_i \right) \xrightarrow{d} (\mathrm{x}_1, \ldots, \mathrm{x}_i), \qquad \text{as } n \to \infty,$$

where $\mathrm{x}_1 > \mathrm{x}_2 > \cdots$ denotes the sequence of the atoms of a Poisson random measure on $(0, \infty)$ with intensity $c\alpha\mu^{-1} e^{-c/\mu} x^{-2} \mathrm{d}x$.

Alternatively, the law of the limiting sequence in Theorems 1 and 2 can be described as follows: for $i \in \mathbb{N}$, $1/\mathrm{x}_1, 1/\mathrm{x}_2 - 1/\mathrm{x}_1, \ldots, 1/\mathrm{x}_i - 1/\mathrm{x}_{i-1}$ are i.i.d. exponential random variables with parameter $c\mu^{-1} e^{-c/\mu}$ in Theorem 1, while in Theorem 2 they are exponential random variables with parameter $c\alpha\mu^{-1} e^{-c/\mu}$.

It is important to point out the similarity with the results for uniform random recursive trees in [3] and preferential attachment trees in [4]. More precisely, the size of the second largest cluster, and more generally, the size of the i-th largest cluster (for $i \geq 2$) in the supercritical regime is of order $n/\ln n$ as in [3] and [4]. Moreover, their sizes are described by the atoms of a Poisson random measure on $(0, \infty)$ whose intensity measure only differ by a constant factor. For example, for uniform random recursive trees [3] the intensity is $ce^{-c} x^{-2} \mathrm{d}x$.

As we mentioned in the introduction, we shall follow a different route to that used in [3] and [4]. The approach developed in this work is based on a remark made in [2, Section 3] about the behavior of the second largest cluster created by performing (supercritical) Bernoulli bond-percolation on complete regular trees. More precisely, consider a rooted complete regular d-ary tree T_h^{d} of height $h \in \mathbb{N}$, where $d \geq 2$ is some integer (i.e., each vertex has exactly out-degree d). Notice that there are d^k vertices at distance $k = 0, 1, \ldots, h$ from the root and a total of $(d^{h+1} - 1)/(d - 1)$ vertices. We then perform Bernoulli bond-percolation with parameter

$$q_h = 1 - ch^{-1} + o(h^{-1}), \tag{4}$$

where $c > 0$ is some fixed parameter. It has been shown in [2, Section 3] that this choice of the percolation parameter corresponds precisely to the supercritical regime, that is, the root cluster is the unique giant component. Because the subtree rooted at a vertex at height $i \leq h$ is again a complete regular d-ary tree with height $h - i$, [2, Corollary 1] essentially shows that the size (number of vertices) G_h^1 of the largest cluster which does not contain the root is close to

$$e^{-c} d^{h-\tau_1(h)+1}/(d - 1),$$

where $\tau_1(h)$ is the smallest height at which an edge has been removed. Notice that there are $d(d^i - 1)/(d - 1)$ edges with height at most i, so the distribution of $\tau_1(h)$ is given by

$$\mathbb{P}(\tau_1(h) > i) = q_h^{d(d^i-1)/(d-1)}, \qquad i = 1, \ldots, h.$$

We use the notation $\log_d x = \ln x/\ln d$ for the logarithm with base d of $x > 0$, and $y = \lfloor y \rfloor + \{y\}$ for the decomposition of a real number y as the sum of its integer and fractional parts. It follows that in the regime (4) and as soon as one assumes $\{\log_d h\} \to \rho \in [0, 1)$, as $h \to \infty$, then $\tau_1(h) - \log_d h$ converges in distribution, and therefore, $hd^{-h}G_h^1$ also converges in distribution.

Our strategy is then to adapt and improve the above argument to study the size of the i-th largest cluster, for $i \geq 2$, in a random split tree with n balls. We also show that this approach can be used to obtain a result similar as Theorem 1 or Theorem 2 for supercritical percolation on complete d-regular trees of height $h \in \mathbb{N}$. More precisely, write G_0 for the number of vertices of the cluster that contains the root and $G_1 \geq G_2 \geq \cdots$ for the sequence of the number vertices of the remaining clusters ranked in decreasing order; for simplicity, we omit the parameter h from our notation. We introduce for every $\rho \in [0, 1)$ a measure Λ_ρ on $(0, \infty)$ by letting

$$\Lambda_\rho([x, \infty)) := d^{-\rho+\lfloor \rho - \log_d x \rfloor + 1}/(d - 1), \qquad x > 0.$$

▶ **Theorem 3.** *Let T_h^{d} be a complete regular d-ary tree of height $h \in \mathbb{N}$ such that $\{\log_d h\} \to \rho \in [0, 1)$, as $h \to \infty$, and suppose that q_h fulfills (4). Then,*

$$d^{-h}G_0 \xrightarrow{d} de^{-c}/(d - 1), \qquad \text{as } h \to \infty,$$

where the constant c is defined in (4). Furthermore, for every fixed $i \in \mathbb{N}$, we have the convergence in distribution

$$(hd^{-h}G_1, \ldots, hd^{-h}G_i) \xrightarrow{d} (\mathrm{x}_1, \ldots, \mathrm{x}_i), \qquad \text{as } h \to \infty,$$

where $\mathrm{x}_1 \geq \mathrm{x}_2 \geq \cdots$ denotes the sequence of the atoms of a Poisson random measure on $(0, \infty)$ with intensity $c\frac{d}{d-1}e^{-c}\Lambda_\rho(\mathrm{d}x)$.

We conclude this extended abstract by providing in Section 2 a fair enough guideline of the proof of Theorem 1. The proofs of Theorem 2 and Theorem 3 follows by an adaptation of the arguments used in the proof of Theorem 1. An important ingredient in the proof of Theorem 1 is Lemma 5 that establishes a law of large number for the number of sub-trees in T_n^{sp} with cardinality (number of balls) larger than $n/\ln n$, which may be of independent interest. Detailed proofs of all our results are going to be given in the complete version [6].

2 Proof of Theorem 1

We split the proof of Theorem 1 in two parts. We start by studying the sizes of percolated sub-trees that are close to the root. One could refer to these percolated sub-trees as the early clusters since their distance to the root is the smallest. Then we show that the largest percolation clusters can be found amongst those (early) percolated sub-trees.

2.1 Sizes of early clusters

For $i \in \mathbb{N}$, let $\mathbf{e}_{i,n}$ be the edge with the i-th smallest height (we break ties by ordering the edges from left to right, however, the order is not relevant in the proofs) that has been removed and $\mathbf{v}_{i,n}$ the endpoint (vertex) of $\mathbf{e}_{i,n}$ that is the furthest away from the root of T_n^{sp}. Let $T_{i,n}$ be the sub-tree of T_n^{sp} that is rooted at $\mathbf{v}_{i,n}$ and let $n_{i,n}$ be the number of balls stored in the sub-tree $T_{i,n}$. For $t \in [0, \infty)$, we write

$$N_n(0) := 0 \quad \text{and} \quad N_n(t) := \sum_{i \geq 1} \mathbb{1}_{\left\{n_{i,n} \geq \frac{n}{t \ln n}\right\}} = \sum_{i \geq 1} \mathbb{1}_{\left\{(n/n_{i,n})^{\frac{1}{\ln n}} \leq t\right\}}$$

for the number of sub-trees $T_{i,n}$ that store more than $\lfloor n/(t \ln n) \rfloor$ balls.

▶ **Theorem 4.** *Suppose that Condition 1 holds and that p_n fulfills (1). Then, the following convergence holds in the sense of weak convergence of finite dimensional distributions,*

$$(N_n(t), t \geq 0) \xrightarrow{d} (N(t), t \geq 0), \qquad \text{as } \; n \to \infty,$$

where $(N(t), t \geq 0)$ is a (classical) Poisson process with intensity $c\mu^{-1}$.

We stress that the convergence in Theorem 4 can be improved in order to show convergence in distribution of the process $(N_n(t), t \geq 0)$ for the Skorohod topology on the space $\mathbb{D}([0, \infty), \mathbb{R})$ of right-continuous functions with left limits to a Poisson process with intensity $c\mu^{-1}$; see, for instance, [8, Theorem 12.6, Chapter 3].

The proof of Theorem 4 uses the following result which provides a law of large number for the number of sub-trees in T_n^{sp} with cardinality larger than $n/\ln n$. More precisely, for a vertex $v \in T_n^{\mathrm{sp}}$ that is not the root $\circ$, let n_v denote the number of balls stored in the sub-tree of T_n^{sp} rooted at v. Define

$$M_n(t) := \# \left\{ v \in T_n^{\mathrm{sp}} : v \neq \circ \; \text{ and } \; n_v \geq \frac{n}{t \ln n} \right\}, \qquad \text{for } \; t \in [0, \infty).$$

▶ **Proposition 5.** *Suppose that Condition 1 holds. Then, for every fixed $t \in [0, \infty)$, we have that $(\ln n)^{-1} M_n(t) \to \mu^{-1} t$, in probability, as $n \to \infty$.*

The proof of Proposition 5 is rather technical and it is given in the complete version [6].

Proof of Theorem 4. For a vertex $v \in T_n^{\mathrm{sp}}$ that is not the root $\circ$, let $\mathbf{e}_v$ be the edge that connects v with its parent. Define the event $E_v := \{$the edge $\mathbf{e}_v$ has been removed after percolation$\}$ and write $\xi_v := \mathbb{1}_{E_v}$. So, $(\xi_v)_{v \neq \circ}$ is a sequence of i.i.d. Bernoulli random variables with parameter $1 - p_n$ (that is, the probability of removing an edge). Then, it should be clear that

$$N_n(t) = \sum_{v \neq \circ} \mathbb{1}_{\left\{n_v \geq \frac{n}{t \ln n}\right\}} \xi_v, \qquad t \in [0, \infty).$$

Let Ω be the σ-algebra generated by $(n_v)_{v\neq\circ}$. Conditioning on Ω, we have that $(N_n(t), t \geq 0)$ has independent increments and that for $0 \leq s \leq t$, $N_n(t) - N_n(s) \stackrel{d}{=} \mathrm{Bin}\left(M_n(t) - M_n(s), 1 - p_n\right)$, where $\mathrm{Bin}(m, q)$ denotes a binomial (m, q) random variable. Therefore, our claim follows from Proposition 5 by appealing to [8, Theorem 12.6, Chapter 3]. ◀

▶ **Corollary 6.** *Suppose that Condition 1 holds and that p_n fulfills (1). Then, for every fixed $i \in \mathbb{N}$, we have the convergence in distribution*

$$\left(\frac{\ln n}{n} n_{1,n}, \dots, \frac{\ln n}{n} n_{i,n}\right) \xrightarrow{d} (\mathrm{x}_1, \dots, \mathrm{x}_i), \qquad as\ \ n \to \infty,$$

where $\mathrm{x}_1 > \mathrm{x}_2 > \cdots$ denotes the sequence of the atoms of a Poisson random measure on $(0, \infty)$ with intensity $c\mu^{-1}x^{-2}\mathrm{d}x$.

Proof. Notice that $(n/n_{1,n})^{\frac{1}{\ln n}} \leq (n/n_{2,n})^{\frac{1}{\ln n}} \leq \cdots$ is the sequence of atoms (or occurrence times) of the counting process $(N_n(t), t \geq 0)$ ranked in increasing order. Then our claim follows directly from Theorem 4, the mapping theorem ([8, Theorem 2.7, Chapter 1]) and basic properties of Poisson random measures (see [26, Proposition 3.7, Chapter 3]). ◀

2.2 Asymptotic sizes of the largest percolation clusters

Recall that, for $i \in \mathbb{N}$, we let $\mathbf{e}_{i,n}$ be the edge with the i-th smallest height that has been removed and $\mathbf{v}_{i,n}$ the endpoint (vertex) of $\mathbf{e}_{i,n}$ that is the furthest away from the root of T_n^{sp}. Recall also that $T_{i,n}$ denotes the sub-tree of T_n^{sp} that is rooted at $\mathbf{v}_{i,n}$ and that we write $n_{i,n}$ for the number of balls stored in the sub-tree $T_{i,n}$. We denote by $\tilde{C}_i$ the size (number of balls) of the root-cluster of $T_{i,n}$ after performing percolation (where here of course root means $\mathbf{v}_{i,n}$). We also write $\tilde{C}_i^*$ for the size (number of balls) of the second largest cluster of $T_{i,n}$ that does not contain its root. In the sequel, we shall use the following notation $A_n = B_n + o_{\mathrm{p}}(f(n))$, where A_n and B_n are two sequences of real random variables and $f : \mathbb{N} \to (0, \infty)$ a function, to indicate that $\lim_{n\to\infty} |A_n - B_n|/f(n) = 0$ in probability.

▶ **Proposition 7.** *Suppose that Condition 1 holds and that p_n fulfills (1). For every fixed $i \in \mathbb{N}$, $\tilde{C}_i^* = o_{\mathrm{p}}(n/\ln n)$. Furthermore, we have the convergence in distribution*

$$\left(\frac{\tilde{C}_1}{n_{1,n}}, \dots, \frac{\tilde{C}_i}{n_{i,n}}\right) \xrightarrow{d} (e^{-c/\mu}, \dots, e^{-c/\mu}), \qquad as\ \ n \to \infty.$$

Proof. Notice that it is enough to show our claim for $i = 1$ since convergence in distribution to a constant is equivalent to convergence in probability, and thus, one can easily deduce the joint convergence for every fixed $i \in \mathbb{N}$. Given $n_{1,n}$, we see that $T_{1,n}$ is a split tree with $n_{1,n}$ balls. Notice that supercritical Bernoulli bond-percolation in $T_{1,n}$ corresponds to a percolation parameter satisfying

$$1 - p_{n_{1,n}} = c/\ln n_{1,n} + o\left(1/\ln n_{1,n}\right),$$

where $c > 0$ is fixed. Notice also that Corollary 6 implies that $(\ln n_{1,n})/\ln n \to 1$, in probability, as $n \to \infty$. Hence $1 - p_{n_{1,n}} = 1 - p_n + o_{\mathrm{p}}\left(1/\ln n\right)$. Therefore, a simple application of [7, Lemma 2] shows that $\tilde{C}_1/n_{1,n} \to e^{-c/\mu}$, in distribution, as $n \to \infty$, which proves the second assertion. Moreover, [7, Lemma 2] also shows that $\tilde{C}_1^*/n_{1,n} \to 0$, in distribution, as $n \to \infty$, and by Corollary 6, we conclude that $\tilde{C}_1^* = o_{\mathrm{p}}(n/\ln n)$. This completes the proof. ◀

▶ **Corollary 8.** *Suppose that Condition 1 holds and that p_n fulfills (1). Then, for every fixed $i \in \mathbb{N}$, we have the convergence in distribution*

$$\left(\frac{\ln n}{n}\tilde{C}_1, \dots, \frac{\ln n}{n}\tilde{C}_i\right) \xrightarrow{d} (\mathrm{x}_1, \dots, \mathrm{x}_i), \qquad \text{as } n \to \infty,$$

where $\mathrm{x}_1 > \mathrm{x}_2 > \cdots$ *denotes the sequence of the atoms of a Poisson random measure on* $(0, \infty)$ *with intensity* $c\mu^{-1}e^{-c/\mu}x^{-2}\mathrm{d}x$.

Proof. This follows from Corollary 6, Proposition 7, the mapping theorem ([8, Theorem 2.7, Chapter 1]) and basic distributional properties of the atoms of Poisson random measures. ◀

The last ingredient in the proof of Theorem 1 consists in verifying that for every fixed $i \in \mathbb{N}$, one can choose $\ell \in \mathbb{N}$ large enough such that with probability tending to 1, as $n \to \infty$, the i-th largest percolation cluster of T_n^{sp} can be found amongst the root-clusters of the percolated tree-components $T_{1,n}, \dots, T_{\ell,n}$. Rigorously, denote by

$$\tilde{C}_{1,\ell} \geq \tilde{C}_{2,\ell} \geq \cdots \geq \tilde{C}_{\ell,\ell}$$

the rearrangement in decreasing order of the $\tilde{C}_i$ for $i = 1, \dots, \ell$. We then adapt the idea of [3, Lemma 6] (details are given in the complete version [6]).

▶ **Lemma 9.** *Suppose that Condition 1 holds and that p_n fulfills (1). Then for each fixed $i \in \mathbb{N}$,*

$$\lim_{\ell \to \infty} \liminf_{n \to \infty} \mathbb{P}\left(\tilde{C}_{k,\ell} = C_k \quad \text{for every } k = 1, \dots, i\right) = 1.$$

We can now finish the proof of Theorem 1.

Proof of Theorem 1. We have already proven the first claim in [7, Lemma 2]. We then only prove the second claim. For every fixed $i \in \mathbb{N}$, consider a continuous function $f : [0, \infty)^i \to [0, 1]$ and fix $\varepsilon > 0$. According to Lemma 9, we may choose $\ell \in \mathbb{N}$ sufficiently large so that there exists $n_\varepsilon \in \mathbb{N}$ such that the upper bound

$$\mathbb{E}\left[f\left(\frac{\ln n}{n}C_1, \dots, \frac{\ln n}{n}C_i\right)\right] \leq \mathbb{E}\left[f\left(\frac{\ln n}{n}\tilde{C}_{1,\ell}, \dots, \frac{\ln n}{n}\tilde{C}_{i,\ell}\right)\right] + \varepsilon$$

holds for all $n \geq n_\varepsilon$. We now deduce from Corollary 8 and the previous bound that

$$\limsup_{n \to \infty} \mathbb{E}\left[f\left(\frac{\ln n}{n}C_1, \dots, \frac{\ln n}{n}C_i\right)\right] \leq \mathbb{E}\left[f\left(\mathrm{x}_1, \dots, \mathrm{x}_i\right)\right] + \varepsilon.$$

Because ε can be arbitrary small and f replaced by $1 - f$, this establishes Theorem 1. ◀

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Scaling and Local Limits of Baxter Permutations Through Coalescent-Walk Processes

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Abstract

Baxter permutations, plane bipolar orientations, and a specific family of walks in the non-negative quadrant are well-known to be related to each other through several bijections. We introduce a further new family of discrete objects, called *coalescent-walk processes*, that are fundamental for our results. We relate these new objects with the other previously mentioned families introducing some new bijections.

We prove joint Benjamini–Schramm convergence (both in the annealed and quenched sense) for uniform objects in the four families. Furthermore, we explicitly construct a new fractal random measure of the unit square, called the *coalescent Baxter permuton* and we show that it is the scaling limit (in the permuton sense) of uniform Baxter permutations.

To prove the latter result, we study the scaling limit of the associated random coalescent-walk processes. We show that they converge in law to a *continuous random coalescent-walk process* encoded by a perturbed version of the Tanaka stochastic differential equation. This result has connections (to be explored in future projects) with the results of Gwynne, Holden, Sun (2016) on scaling limits (in the Peanosphere topology) of plane bipolar triangulations.

We further prove some results that relate the limiting objects of the four families to each other, both in the local and scaling limit case.

2012 ACM Subject Classification Mathematics of computing → Probability and statistics; Mathematics of computing → Permutations and combinations

Keywords and phrases Local and scaling limits, permutations, planar maps, random walks in cones

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.7

Related Version A full version of this extended abstract will be submitted later to another journal.

Acknowledgements Thanks to Mathilde Bouvel, Valentin Féray and Grégory Miermont for their dedicated supervision and enlightening discussions. Thanks to Nicolas Bonichon, Emmanuel Jacob, Jason Miller, Kilian Raschel, Olivier Raymond, Vitali Wachtel, for enriching discussions and pointers.

1 Introduction and main results

Baxter permutations were introduced by Glen Baxter in 1964 [3] to study fixed points of commuting functions. *Baxter permutations* are permutations avoiding the two vincular patterns $2\,\underline{41}\,3$ and $3\,\underline{14}\,2$, i.e. permutations σ such that there are no indices $i < j < k$ such that $\sigma(j+1) < \sigma(i) < \sigma(k) < \sigma(j)$ or $\sigma(j) < \sigma(k) < \sigma(i) < \sigma(j+1)$.

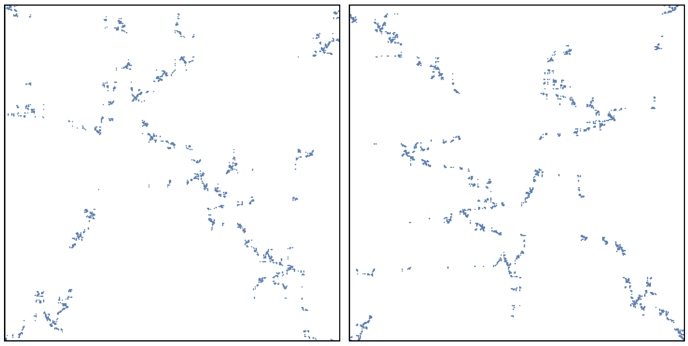

Figure 1 The diagrams of two uniform Baxter permutations of size 3253 (left) and 4520 (right). (How these permutations were obtained is discussed in Appendix C).

In the last 30 years, several bijections between Baxter permutations, plane bipolar orientations and certain walks in the plane[1] have been discovered. These relations between discrete objects of different nature are a *beautiful piece of combinatorics*[2] that we aim at investigating from a more probabilistic point of view in this extended abstract. The goal of our work is to explore local and scaling limits of these objects and to study the relations between their limits. Indeed, since these objects are related by several bijections at the discrete level, we expect that most of the relations among them also hold in the "limiting discrete and continuous worlds".

We mention that some limits of these objects (and related ones) were previously investigated. Dokos and Pak [11] explored the expected limit shape of doubly alternating Baxter permutations, i.e. Baxter permutations σ such that σ and σ^{-1} are alternating. In their article they claimed that *"it would be interesting to compute the limit shape of random Baxter permutations"*. One of the main goals of our work is to answer this question by proving permuton convergence for uniform Baxter permutations (see Theorem 5 below). For plane walks (i.e. walks in $\mathbb{Z}^2$) conditioned to stay in a cone, we mention the remarkable works of Denisov and Wachtel [10] and Duraj and Wachtel [12] where they proved (together with many other results) convergence towards Brownian meanders or excursions in cones. This allowed Kenyon, Miller, Sheffield and Wilson [19] to show that the quadrant walks encoding uniformly random plane bipolar orientations (see Section 2.2 for more details) converge to a Brownian excursion of correlation $-1/2$ in the quarter-plane. This is interpreted as Peanosphere convergence of the maps decorated by the *Peano curve* (see Section 2.2 for further details) to a $\sqrt{4/3}$-Liouville Quantum Gravity (LQG) surface decorated by an independent SLE_{12}. This result was then significantly strengthened by Gwynne, Holden and Sun [14] who proved joint convergence for the map and its dual, in the setting of infinite-volume triangulations. In proving Theorem 5 we extend some of the methods and results of [14], with a key difference in the way limiting objects are defined. We discuss this in more precise terms at the end of this introduction.

So far we have considered three families of objects: Baxter permutations (denoted by $\mathcal{P}$); walks in the non-negative quadrant ($\mathcal{W}$) starting on the y-axis and ending on the x-axis, with some specific admissible increments defined in the forthcoming Equation (4); and plane bipolar orientations ($\mathcal{O}$). For our purposes, specifically for the proof of the permuton convergence, we introduce in Section 2.4 a fourth family of objects called *coalescent-walk processes* ($\mathcal{C}$).

[1] We refer to Section 2 for a precise definition of all these objects.
[2] Quoting the abstract of [13].

We denote by $\mathcal{W}_n$ the subset of $\mathcal{W}$ consisting of quadrant walks of size n (and similarly $\mathcal{C}_n, \mathcal{P}_n, \mathcal{O}_n$ for the other three families). We will present four size-preserving bijections (denoted using two letters that refer to the domain and co-domain) between these four families, summarized in the following diagram:

$$\begin{tikzcd} \mathcal{W} \arrow[r, "\mathrm{WC}"] & \mathcal{C} \arrow[d, "\mathrm{CP}"] \\ \mathcal{O} \arrow[u, "\mathrm{OW}"] \arrow[r, "\mathrm{OP}"] & \mathcal{P} \end{tikzcd}, \tag{1}$$

where the mapping OW was introduced in [19] and OP in [5]; the others are new. Our first result is the following:

▶ **Theorem 1.** *The diagram in Equation* (1) *commutes. In particular,* $\mathrm{CP} \circ \mathrm{WC} : \mathcal{W} \to \mathcal{P}$ *is a size-preserving bijection.*

Our second result deals with local limits, more precisely Benjamini–Schramm limits. Informally, Benjamini–Schramm convergence for discrete objects looks at the convergence of the neighborhoods (of any fixed size) of a uniformly distinguished point of the object (called root). In order to properly define the Benjamini–Schramm convergence for the four families, we need to present the respective local topologies. We defer this task to the complete version of this abstract, here we just mention that the local topology for graphs (and so plane bipolar orientations) was introduced by Benjamini and Schramm [4] while the local topology for permutations was introduced by the first author [6]. Local topologies for plane walks and coalescent-walk processes can be defined in a similar way. We denote by $\widetilde{\mathfrak{W}}_\bullet$ the completion of the space of rooted walks $\bigsqcup_{n\geq 1} \mathcal{W}_n \times [n]$ with respect to the metric defining the local topology. The spaces $\widetilde{\mathfrak{C}}_\bullet, \widetilde{\mathfrak{S}}_\bullet, \widetilde{\mathfrak{m}}_\bullet$ are defined likewise from $\mathcal{C}, \mathcal{P}, \mathcal{O}$.

We define below the candidate limiting objects. As a matter of fact, a formal definition requires an extension of the mappings in Equation (1) to infinite-volume objects (for the mappings WC and OW^{-1} also an extension to walks that are *not* conditioned in the quadrant). We do not present all the details of such extensions, but they can be easily guessed from our description of the mappings WC, OW, CP and OP given in Section 2.

Let ν denote the probability distribution on $\mathbb{Z}^2$ given by:

$$\nu = \frac{1}{2}\delta_{(+1,-1)} + \sum_{i,j\geq 0} 2^{-i-j-3}\delta_{(-i,j)}, \quad \text{where } \delta \text{ denotes the Dirac measure,} \tag{2}$$

and let[3] $\bar{\boldsymbol{W}} = (\bar{\boldsymbol{X}}, \bar{\boldsymbol{Y}}) = (\bar{\boldsymbol{W}}_t)_{t\in\mathbb{Z}}$ be a bidirectional random plane walk with step distribution ν, with value $(0,0)$ at time 0. Let $\bar{\boldsymbol{Z}} = \mathrm{WC}(\bar{\boldsymbol{W}})$ be the corresponding infinite coalescent-walk process, $\bar{\boldsymbol{\sigma}} = \mathrm{CP}(\bar{\boldsymbol{Z}})$ the corresponding infinite permutation on $\mathbb{Z}$ (in this context, an infinite permutation is a total order of $\mathbb{Z}$), and $\bar{\boldsymbol{m}} = \mathrm{OW}^{-1}(\bar{\boldsymbol{W}})$ the corresponding infinite map.

▶ **Theorem 2.** *For every $n \in \mathbb{Z}_{>0}$, let $\boldsymbol{W}_n$, $\boldsymbol{Z}_n$, $\boldsymbol{\sigma}_n$, and $\boldsymbol{m}_n$ denote uniform objects of size n in $\mathcal{W}_n$, $\mathcal{C}_n$, $\mathcal{P}_n$, and $\mathcal{O}_n$ respectively, related by the bijections of Equation* (1)*. For every $n \in \mathbb{Z}_{>0}$, let $\boldsymbol{i}_n$ be an independently chosen uniform index of $[n]$. Then we have joint convergence in distribution in the space $\widetilde{\mathfrak{W}}_\bullet \times \widetilde{\mathfrak{C}}_\bullet \times \widetilde{\mathfrak{S}}_\bullet \times \widetilde{\mathfrak{m}}_\bullet$:*

$$((\boldsymbol{W}_n, \boldsymbol{i}_n), (\boldsymbol{Z}_n, \boldsymbol{i}_n), (\boldsymbol{\sigma}_n, \boldsymbol{i}_n), (\boldsymbol{m}_n, \boldsymbol{i}_n)) \xrightarrow[n\to\infty]{d} (\bar{\boldsymbol{W}}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{\sigma}}, \bar{\boldsymbol{m}}).$$

[3] Here and throughout the paper we denote random quantities using **bold** characters.

▶ Remark 3. We give a few comments on this result.

1. The mapping OW^{-1} naturally endows the map $\boldsymbol{m}_n$ with an edge labeling and the root $\boldsymbol{i}_n$ of $\boldsymbol{m}_n$ is chosen according to this labeling.
2. We can also prove a quenched version of the above result (of annealed type) for all the four objects (not presented in this extended abstract). It entails (see [6, Theorem 2.32]) that consecutive pattern densities of $\boldsymbol{\sigma}_n$ jointly converge in distribution.
3. The fact that the four convergences are joint follows from the fact that the extensions of the mappings in Equation (1) to infinite-volume objects are a.s. continuous.

Our third (and main) result is a scaling limit result for Baxter permutations (see Figure 1 for some simulations), in the framework of permutons developed by [17]. A *permuton* μ is a Borel probability measure on the unit square $[0,1]^2$ with uniform marginals, that is $\mu([0,1]\times[a,b]) = \mu([a,b]\times[0,1]) = b-a$, for all $0 \leq a \leq b \leq 1$. Any permutation σ of size $n \geq 1$ may be interpreted as the permuton μ_σ given by the sum of Lebesgue area measures

$$\mu_\sigma(A) = n\sum_{i=1}^{n} \mathrm{Leb}\big([(i-1)/n, i/n]\times[(\sigma(i)-1)/n, \sigma(i)/n]\cap A\big), \tag{3}$$

for all Borel measurable sets A of $[0,1]^2$. Let $\mathcal{M}$ be the set of permutons. As for general probability measure, we say that a sequence of (deterministic) permutons $(\mu_n)_n$ converges *weakly* to μ (simply denoted $\mu_n \to \mu$) if $\int_{[0,1]^2} f d\mu_n \to \int_{[0,1]^2} f d\mu$, for every (bounded and) continuous function $f:[0,1]^2 \to \mathbb{R}$. With this topology, $\mathcal{M}$ is compact. Convergence for random permutations is defined as follows:

▶ **Definition 4.** *We say that a random permutation $\boldsymbol{\sigma}_n$ converges in distribution to a random permuton $\boldsymbol{\mu}$ as $n \to \infty$ if the random permuton $\mu_{\boldsymbol{\sigma}_n}$ converges in distribution to $\boldsymbol{\mu}$ with respect to the weak topology.*

Random permuton convergence entails joint convergence in distribution of all (classical) pattern densities (see [1, Theorem 2.5]). The study of permuton limits, as well as other scaling limits of permutations, is a rapidly developing field in discrete probability theory, see for instance [1, 2, 7, 8, 16, 18, 20, 21, 22]. Our main result is the following:

▶ **Theorem 5.** *Let $\boldsymbol{\sigma}_n$ be a uniform Baxter permutation of size n. There exists a random permuton $\boldsymbol{\mu}_B$ such that $\mu_{\boldsymbol{\sigma}_n} \xrightarrow{d} \boldsymbol{\mu}_B$.*

An explicit construction of the limiting permuton $\boldsymbol{\mu}_B$, called the *coalescent Baxter permuton*, is given in Section 3.2. The proof of Theorem 5 is based on a result on scaling limits of the coalescent-walk processes $\boldsymbol{Z}_n$, which appears to be of independent interest, and is discussed in Section 3.1. In particular, the convergence of uniform Baxter permutations is joint[4] with that of the conditioned versions of $\boldsymbol{W}_n$ and $\boldsymbol{Z}_n$ presented in Theorem 26.

We finally discuss the relations with the work of Gwynne, Holden and Sun [14]. They show that for infinite-volume bipolar oriented triangulations, the explorations of the two tree/dual tree pairs of the map and its dual converge jointly. The limit is the pair of planar Brownian motions which encode the same $\sqrt{4/3}$-LQG surface decorated by both an SLE_{12} curve and the "dual" SLE_{12} curve, traveling in a direction perpendicular (in the sense of imaginary geometry) to the original curve. As shown below (Lemma 12), the bijection of [5]

[4] We leave a proper claim of joint convergence to the full version of this paper. However the joint distribution of the scaling limits is the one presented in Section 3.2.

between plane bipolar orientations and Baxter permutations can be rewritten in terms of the interaction of these two tree/dual tree pairs, which explains the connection between our work and the one of [14].

We prove Theorem 5 by extending some of their constructions to finite-volume general maps, which allows us to provide an analog of their result (that are restricted to triangulations) for general plane bipolar orientations in finite volume, jointly with the convergences above[5]. More precisely, the coalescent-walk process defined in Section 2.4.1 is an extension of the random walk $\mathcal{X}$ defined in [14, Section 2.1]. The fact that it encodes the spanning tree of the dual map (Proposition 19) is a version of [14, Lemma 2.1], albeit we present it differently. Our main technical ingredient is the convergence of the coalescent-walk process driven by a random plane walk of Theorem 24. It corresponds to [14, Theorem 4.1]. The way the limiting object (the right-hand side of Equation (10)) is defined is however very different, and the proofs differ as a consequence. In our case, it comes from a stochastic differential equation (Equation (7)), for which existence and uniqueness are known from the literature [9, 23]. In their case, it is built using imaginary geometry, and characterized by its excursion decomposition. These are nonetheless two descriptions of the same object, providing an SDE formulation of an intricate imaginary geometry coupling. We wish to explore consequences of this in further works.

Outline of the extended abstract. The remainder of the abstract is organized as follows. In Section 2 we present the objects and the mappings involved in the diagram in Equation (1). Moreover, we sketch the proof of Theorem 1. Section 3 is devoted to developing the theory for the proof of Theorem 5. In particular, in Section 3.1 we present the aforementioned results for scaling limits of coalescent-walk processes, and in Section 3.2 we give an explicit construction of the limiting permuton for Baxter permutations. Finally, in Appendix A we prove our main technical ingredient (Theorem 24), and in Appendix B we finish the proof of Theorem 5. Note that we leave the proof of Theorem 2 out of this abstract.

2 Bipolar orientations, walks in the non-negative quadrant, Baxter permutations and coalescent-walk processes

2.1 Plane bipolar orientations

We recall that a *planar map* is a connected graph embedded in the plane with no edge-crossings, considered up to continuous deformation. A map has vertices, edges, and faces, the latter being the connected components of the plane remaining after deleting the edges. The outer face is unbounded, the inner faces are bounded.

▶ **Definition 6.** *A* plane bipolar orientation *(or simply* bipolar orientation*) is a planar map with oriented edges such that*

- *there are no oriented cycles;*
- *there is exactly one vertex with only outgoing edges (the source, denoted s), and exactly one vertex with only incoming edges (the sink, denoted s'); all other vertices, called non-polar, have both types of edges;*
- *the source and the sink are both incident to the outer face.*

The size of a bipolar orientation m is its number of edges and will be denoted with $|m|$.

[5] Not presented in this extended abstract.

Every bipolar orientation can be plotted in the plane in such a way that every edge is oriented from bottom to top (as done for example in Figure 2).

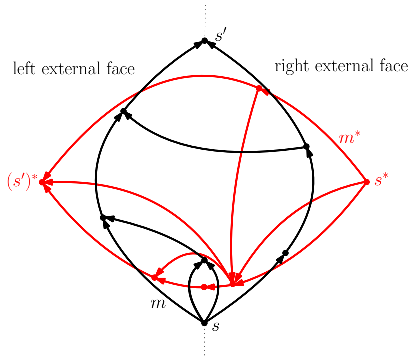

Figure 2 In black, a bipolar orientation m of size 10. Note that every edge is oriented from bottom to top. In red, its dual map m^*. Similarly, we plot the dual map in such a way that every edge is oriented from right to left. This map will be used in several examples. In later pictures, the orientation of each edge is not displayed.

Given a bipolar orientation, an edge e from v to w is bordered, in the clockwise cyclic order, by its bottom vertex, its left face, its top vertex, its right face. It is useful, for the consistency of definitions, to think of the external face as split in two (see Figure 2 for an example): the *left external face*, and the *right external face*.

There is a natural notion of duality for a bipolar orientation m. It is the classical duality for (unoriented) maps where the orientation of a dual edge between two primal faces is from right to left. The primal right external face becomes the dual source, and the primal left external face becomes the dual sink. This map m^* is also a bipolar orientation (see Figure 2). The map m^{**} is just the reversal of the map m: the source and sink are exchanged, and all edges are reversed.

Given a bipolar orientation m, its *down-right tree* $T(m)$ may be defined as a set of edges equipped with a parent relation, as follows.

- The edges of $T(m)$ are the edges of m.
- Let $e \in m$ and v its bottom vertex.
  - If v is the source, then e has no parent edge in $T(m)$ (it is grafted to the root of $T(m)$);
  - if v is not the source, the parent edge of e in $T(m)$ is the right-most incoming edge of v.

The tree $T(m)$ can be drawn on top of m: the root of $T(m)$ corresponds to the source s of m, internal vertices of $T(m)$ correspond to non-polar vertices of m, and leaves of $T(m)$ are the midpoints of some edges of m. Note that one can draw the trees $T(m)$ and $T(m^{**})$ on the map m without any crossing (see the left-hand side of Figure 3 for an example).

We conclude this section recalling that the *exploration* of a tree T is the visit of its vertices (or its edges) following the contour of the tree in the clockwise order.

2.2 Kenyon-Miller-Sheffield-Wilson bijection

We now present a bijection between bipolar orientations and some walks in the non-negative quadrant $\mathbb{Z}^2_{\geq 0}$, introduced in [19, Section 2] by Kenyon, Miller, Sheffield and Wilson.

Let m be a bipolar orientation. We consider the exploration of the tree $T(m)$ (highlighted in green in the middle picture of Figure 3) starting at the source s and ending at the last visit of the sink s'. Note that this path (when reversed) is also the exploration of the tree

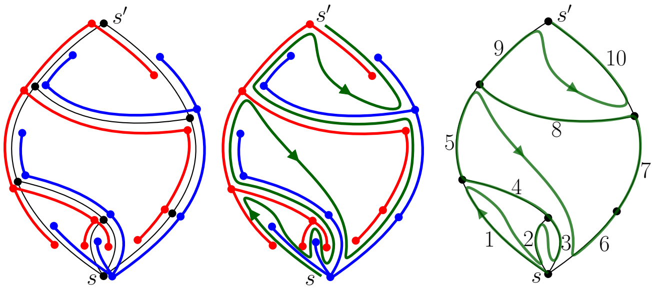

Figure 3 Left: A bipolar orientation m with the trees $T(m)$ (in blue) and $T(m^{**})$ (in red). **Middle:** We add in green the *interface path* tracking the interface between the two trees (see Section 2.2). **Right:** We label the edges of the bipolar orientations following the interface path.

$T(m^{**})$ stopped at the last visit of the source s. This path, called *interface path*[6] since it winds between the trees $T(m)$ and $T(m^{**})$, identifies an ordering on the set E of edges of m since every edge of $T(m)$ corresponds exactly to one edge of m (see the right-hand side of Figure 3 for an example). Let $e_1, e_2, \dots, e_{|m|}$ be the edges of m listed according to this order.

▶ **Definition 7.** *Given a bipolar orientation m, the corresponding walk* $\mathrm{OW}(m) = (W_t)_{t\in[|m|]} = (X_t, Y_t)_{t\in[|m|]}$ *of size $|m|$ in the non-negative quadrant $\mathbb{Z}^2_{\geq 0}$ is defined as follows: for $t \in [|m|]$, let X_t be the distance in the tree $T(m)$ between the bottom vertex of e_t and the root of $T(m)$ (corresponding to the source s), and let Y_t be the distance in the tree $T(m^{**})$ between the top vertex of e_t and the root of $T(m^{**})$ (corresponding to the sink s').*

▶ Remark 8. The walk $(0, X_1 + 1, \dots, X_{|m|} + 1)$ is the height process of the tree $T(m)$. The walk $(0, Y_{|m|} + 1, Y_{|m|-1} + 1, \dots, Y_1 + 1)$ is the height process of the tree $T(m^{**})$.

Suppose that the left external face has $h + 1$ edges and the right external face has $k + 1$ edges, for some $h, k \geq 0$. Then the walk $(W_t)_{1\leq t\leq|m|}$ starts at $(0, h)$, ends at $(k, 0)$, and stays in the non-negative quadrant $\mathbb{Z}^2_{\geq 0}$. We finally investigate the possible values for the increments of the walk, i.e. the values of $W_{t+1} - W_t$. We say that two edges of a tree are consecutive if one is the parent of the other. We first highlight that the interface path of the map m has two different behaviors when following the edges e_t and e_{t+1}:

- either it is following two consecutive edges of $T(m)$ (this is the case, for instance, of the edges e_3 and e_4 on the right-hand side of Figure 3);
- or it is first following e_t, then it is traversing a face of m, and finally is following e_{t+1} (this is the case, for instance, of the edges e_5 and e_6 on the right-hand side of Figure 3).

When the latter case happens, the interface path splits the boundary of the traversed face in two parts, a left and a right boundary.

Therefore the increments of the walk are either $(+1, -1)$ (when e_t and e_{t+1} are consecutive) or $(-i, +j)$, for some $i, j \in \mathbb{Z}_{\geq 0}$ (when, between e_t and e_{t+1}, the interface path is traversing a face with $i + 1$ edges on the left boundary and $j + 1$ edges on the right boundary). We denote by A the set of possible increments, that is

$$A = \{(+1, -1)\} \cup \{(-i, j), i \in \mathbb{Z}_{\geq 0}, j \in \mathbb{Z}_{\geq 0}\}. \tag{4}$$

We denote by $\mathcal{W}$ the set of walks in the non-negative quadrant, starting at $(0, h)$ and ending at $(k, 0)$ for some $h \geq 0, k \geq 0$, with increments in A.

[6] The interface path goes sometimes under the name of *Peano curve*, see for instance [15].

▶ **Theorem 9** ([19, Theorem 1]). *The mapping* $\mathrm{OW} : \mathcal{O} \to \mathcal{W}$ *is a size-preserving bijection.*

▶ **Example 10.** We consider the map m in Figure 3. The corresponding walk $\mathrm{OW}(m)$ is:

$$\Big((0,2),(0,3),(0,3),(1,2),(2,1),(0,3),(1,2),(2,1),(3,0),(2,0)\Big).$$

2.3 Baxter permutations and bipolar orientations

In [5], a bijection between Baxter permutations and bipolar orientations is given. We give here a slightly different formulation of this bijection (more convenient for our purposes) and then in Lemma 12 we state that the two formulations are equivalent.

▶ **Definition 11.** *Let* m *be a bipolar orientation of size* $n \geq 1$*. Recall that to every edge of the map* m *corresponds its dual edge in the dual map* m^**. The Baxter permutation* $\mathrm{OP}(m)$ *associated with* m *is the only permutation* π *such that for every* $1 \leq i \leq n$*, the* i*-th edge visited in the exploration of* $T(m)$ *corresponds to the* $\pi(i)$*-th edge visited in the exploration of* $T(m^*)$*. We say that this edge corresponds to the index* i*.*

An example is given in Figure 4. The following result proves that OP is a bijection.

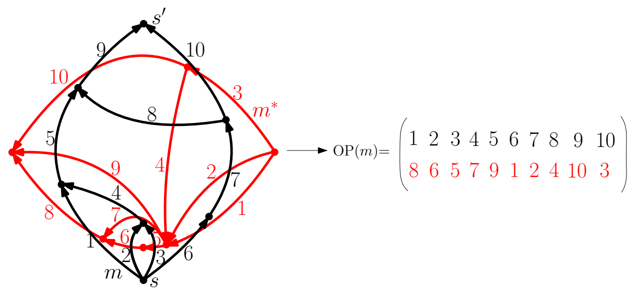

Figure 4 Left: The bipolar orientation m and its dual m^*, already considered in Figure 2. We plot in black the labeling of the edges of m obtained in Figure 3 and in red the labeling of the edges of m^* obtained using the same procedure used for m. **Right:** The permutation $\mathrm{OP}(m)$ obtained by pairing the labels of the corresponding primal and dual edges between m and m^*.

▶ **Lemma 12.** *The function* $\mathrm{OP} : \mathcal{O} \to \mathcal{P}$ *is equal to the function* $\Psi : \mathcal{O} \to \mathcal{P}$ *defined in [5, Section 3.2]. Therefore* OP *is a size-preserving bijection.*

The definition of Ψ is the same as that of OP, with $T(m^*)$ replaced by $T(m^{-1})$, m^{-1} denoting the symmetry of m along the vertical axis. So the proof (that we omit) amounts to showing that these two trees visit the edges of m in the same order[7].

2.4 Discrete coalescent-walk processes

Since the key ingredient for permuton convergence is the extraction of patterns (see Proposition 32), we introduce in this section a new tool in order to "extract patterns from the plane walk" that encodes a Baxter permutation, namely *coalescent-walk processes*. Then, in Section 2.4.1, we present a bijection between walks in the non-negative quadrant and

[7] Actually they are related by a classic bijection between trees: the Lukasiewicz walk of $T(m^*)$ is the reversal of the height function of $T(m^{-1})$.

a specific kind of coalescent-walk processes, and in Section 2.4.2, we introduce a bijection between these coalescent-walk processes and Baxter permutations. Composing these two mappings we obtain another bijection between walks in the non-negative quadrant and Baxter permutations. Finally, in Section 2.5 we complete the proof of Theorem 1.

▶ **Definition 13.** *Let I be a (finite or infinite) interval of $\mathbb{Z}$. We call* coalescent-walk process *over I a family $\{(Z^{(t)}_s)_{s\geq t, s\in I}\}_{t\in I}$ of one-dimensional walks such that*

- *the walk $Z^{(t)}$ starts at zero at time t, i.e. $Z^{(t)}_t = 0$;*
- *if $Z^{(t)}_k \geq Z^{(t')}_k$ (resp. $Z^{(t)}_k \leq Z^{(t')}_k$) at some time k, then $Z^{(t)}_{k'} \geq Z^{(t')}_{k'}$ (resp. $Z^{(t)}_{k'} \leq Z^{(t')}_{k'}$) for every $k' \geq k$.*

Note that, as a consequence, if $Z^{(t)}_k = Z^{(t')}_k$, at time k, then $Z^{(t)}_{k'} = Z^{(t')}_{k'}$ for every $k' \geq k$. In this case, we say that $Z^{(t)}$ and $Z^{(t')}$ are *coalescing* and call *coalescent point* of $Z^{(t)}$ and $Z^{(t')}$ the point $(\ell, Z^{(t)}_\ell)$ such that $\ell = \min\{k \geq \max\{t,t'\} | Z^{(t)}_k = Z^{(t')}_k\}$. We denote by $\mathfrak{C}(I)$ the set of coalescent-walk processes over some interval I.

2.4.1 The coalescent-walk process corresponding to a plane walk

We now introduce a particular family of coalescent-walk processes of interest for us. Let I be a (finite or infinite) interval of $\mathbb{Z}$. Recall the definition of A from Equation (4) page 7, and let $\mathfrak{W}_A(I)$ be the set of plane walks of time space I (functions $I \to \mathbb{Z}^2$) with increments in A.

Take $W \in \mathfrak{W}_A(I)$ and denote $W_t = (X_t, Y_t)$ for $t \in I$. From X and Y we construct the family of walks $\{Z^{(t)}\}_{t\in I}$, called the coalescent-walk process associated with W, by

- for $t \in I$, $Z^{(t)}_t = 0$;
- for $t \in I$ and $k \in I \cap [t+1, +\infty)$,

$$Z^{(t)}_k = \begin{cases} Z^{(t)}_{k-1} + (Y_k - Y_{k-1}), & \text{if } \; Z^{(t)}_{k-1} \geq 0, \\ Z^{(t)}_{k-1} - (X_k - X_{k-1}), & \text{if } \; Z^{(t)}_{k-1} < 0 \text{ and } Z^{(t)}_{k-1} - (X_k - X_{k-1}) < 0, \\ Y_k - Y_{k-1}, & \text{if } \; Z^{(t)}_{k-1} < 0 \text{ and } Z^{(t)}_{k-1} - (X_k - X_{k-1}) \geq 0. \end{cases} \tag{5}$$

Let $\mathrm{WC} : \mathfrak{W}_A(I) \to \mathfrak{C}(I)$ map each $W \in \mathfrak{W}_A(I)$ to the corresponding coalescent-walk process, i.e. $\mathrm{WC}(W) = \{Z^{(t)}\}_{t\in I}$. We also set $\mathcal{C}_n = \mathrm{WC}(\mathcal{W}_n) \subset \mathfrak{C}([n])$ and $\mathcal{C} = \cup_{n\in\mathbb{Z}_{\geq 0}} \mathcal{C}_n$.

We give a heuristic explanation of this construction in the following example.

▶ **Example 14.** We consider the plane walk $W = (W_t)_{t\in[10]}$ starting at $(0,0)$ on the left-hand side of Figure 5. We plot in the second diagram of Figure 5 the walks Y in red and $-X$ in blue. We now explain how we reconstruct the ten walks $\{Z^{(t)}\}_{1\leq t\leq 10}$ (in green on the right-hand side of Figure 5). The walk $Z^{(t)}$ starts at height zero at time t. Then,

- If $Z^{(t)}_{k-1}$ is non-negative (in particular at the starting point), then the increment $Z^{(t)}_k - Z^{(t)}_{k-1}$ is the same as the one of the red walk.
- If $Z^{(t)}_{k-1}$ is negative, then the increment $Z^{(t)}_k - Z^{(t)}_{k-1}$ is the same as the one of the blue walk, as long as this increment keeps $Z^{(t)}_k$ negative.
- Now if at time $k-1$, $Z^{(t)}_{k-1}$ is negative but the blue increment would "force" it to cross (or touch) the x-axis (that is if $X_k - X_{k-1} \leq Z^{(t)}_{k-1} < 0$), then $Z^{(t)}_k$ is equal to $Y_k - Y_{k-1}$ (i.e. $Z^{(t)}$ coalesces with $Z^{(k-1)}$ at time k). For instance this is the case of the second increment of the walk $Z^{(7)}$.

▶ **Observation 15.** *The y-coordinates of the coalescent points of a coalescent-walk process in $\mathcal{C}(I)$ are non-negative.*

2.4.2 The permutation associated with a coalescent-walk process

Given a coalescent-walk process $Z = \{Z^{(t)}\}_{t\in I}$ defined on a (finite or infinite) interval I, the relation $\leq_Z$ on I defined as follows is a total order (we skip the proof of this fact):

$$i \leq_Z j \quad \iff \quad \{i < j \text{ and } Z_j^{(i)} < 0\} \quad \text{or} \quad \{j < i \text{ and } Z_i^{(j)} \geq 0\} \quad \text{or} \quad \{i = j\}. \qquad (6)$$

This definition allows to associate a permutation to a coalescent-walk process.

▶ **Definition 16.** *Fix $n \in \mathbb{Z}_{\geq 0}$. Let $Z = \{Z^{(t)}\}_{t\in[n]} \in \mathcal{C}_n$ be a coalescent-walk process over $[n]$. Denote $\mathrm{CP}(Z)$ the permutation $\sigma \in \mathfrak{S}_n$ such that for $1 \leq i,j \leq n$, $\sigma(i) \leq \sigma(j) \iff i \leq_Z j$.*

We have that pattern extraction in the permutation $\mathrm{CP}(Z)$ depends only on a finite number of trajectories, a key step towards proving permuton convergence.

▶ **Proposition 17.** *Let σ be a permutation obtained from a coalescent-walk process $Z = \{Z^{(t)}\}_{t\in[n]}$ via the map CP. Let $I = \{i_1 < \cdots < i_k\} \subset [n]$. Then[8] $\mathrm{pat}_I(\sigma) = \pi$ if the following condition holds: for all $1 \leq \ell < s \leq k$, $Z_{i_s}^{(i_\ell)} \geq 0 \iff \pi(s) < \pi(\ell)$.*

We end this section with the following observation. Note that given a coalescent-walk process on $[n]$, the plane drawing of the trajectories $\{Z^{(t)}\}_{t\in I}$ identifies a natural tree structure $\mathrm{Tr}(Z)$ as follows (see for instance the middle and right-hand side of Figure 6):

- vertices of $\mathrm{Tr}(Z)$ correspond to points $1,\ldots,n$ on the x-axis, plus a root.
- Edges are portions of trajectories starting at the right of a vertex i and interrupted at the first encountered new vertex. Trajectories that do not encounter a new vertex before time n are connected to the root. The label i is also carried by the edge at the right of i.

▶ Remark 18. In the case where $I = [n]$ for some $n \in \mathbb{Z}_{\geq 0}$, the permutation $\pi = \mathrm{CP}(Z)$ is readily obtained from $\mathrm{Tr}(Z)$: it is enough to label the points $1,\ldots,n$ on the x-axis of the diagram of the colaescent-walk process Z (these labels are painted in purple in the middle picture of Figure 6) according to the exploration process of $\mathrm{Tr}(Z)$ and then to read these labels from left to right.

2.5 From plane walks to Baxter permutations via coalescent-walk processes

We sketch here the proof of Theorem 1. The key ingredient is to show that the dual tree $T(m^*)$ of a bipolar orientation can be recovered from its encoding plane walk by building the associated coalescent-walk process Z and looking at the corresponding tree $\mathrm{Tr}(Z)$. More

[8] See Appendix B for notation on patterns of permutations.

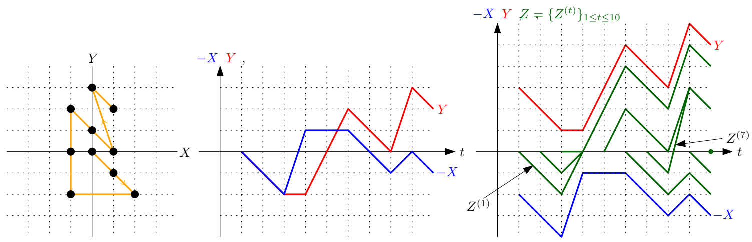

Figure 5 Left: A plane walk (X, Y) starting at (0,0). **Middle:** The diagram of the walks Y (in red) and $-X$ (in blue). **Right:** The two walks are shifted (one towards the top and one to the bottom) and the ten walks of the coalescent-walk process are plotted in green.

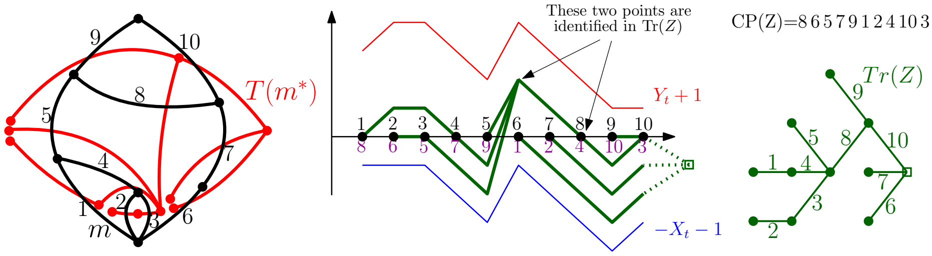

Figure 6 On the left-hand side the map m from Figure 4. In the middle the associated coalescent-walk process $Z = \mathrm{WC} \circ \mathrm{OW}(m)$ that naturally determines the tree $\mathrm{Tr}(Z)$ (shown on the right). Note that the exploration of $\mathrm{Tr}(Z)$ gives the inverse permutation $\mathrm{CP}(Z)^{-1} = 6\,7\,10\,8\,3\,2\,4\,1\,5\,9$.

precisely, let $W = (W_t)_{1 \le t \le n} = \mathrm{OW}(m)$ be the walk encoding a given bipolar orientation m, and $Z = \mathrm{WC}(W)$ be the corresponding coalescent-walk process. Then the following result, illustrated by an example in Figure 6, holds.

▶ **Proposition 19.** *The tree $\mathrm{Tr}(Z)$ is equal to the dual tree $T(m^*)$ with edges labeled according to the order given by the exploration of $T(m)$.*

The proof requires a lot more notation so we skip it in this extended abstract. Theorem 1 then follows immediately, by construction of $\mathrm{OP}(m)$ from $T(m^*)$ and $T(m)$ (Definition 11) and of $\mathrm{CP}(Z)$ from $\mathrm{Tr}(Z)$ (Remark 18).

3 Convergence to the Baxter permuton

We start this section by representing a uniform random walk in $\mathcal{W}_n$ as a conditioned random walk. For all $n \geq 2$, let $\mathfrak{W}_n^{A,\mathrm{exc}}$ be the set of plane walks $(W_t)_{0 \le t \le n-1}$ of length n that stay in the non-negative quadrant, starting and ending at $(0,0)$, with increments in A (defined in Equation (4)). Remark that for $n \geq 1$, the mapping $\mathfrak{W}_{n+2}^{A,\mathrm{exc}} \to \mathcal{W}_n$ removing the first and the last step, i.e. $W \mapsto (W_t)_{1 \le t \le n}$, is a bijection. Recall also that $\bar{\boldsymbol{W}}$ denotes the walk defined below Equation (2). An easy calculation then gives the following (observed also in [19, Remark 2]):

▶ **Proposition 20.** *Conditioning on $\{(\bar{\boldsymbol{W}}_t)_{0 \le t \le n+1} \in \mathfrak{W}_{n+2}^{A,\mathrm{exc}}\}$, the law of $(\bar{\boldsymbol{W}}_t)_{0 \le t \le n+1}$ is the uniform distribution on $\mathfrak{W}_{n+2}^{A,\mathrm{exc}}$, and the law of $(\bar{\boldsymbol{W}}_t)_{1 \le t \le n}$ is the uniform distribution on $\mathcal{W}_n$.*

As we said in the introduction, a key result to prove Theorem 5 is to determine the scaling limit of coalescent-walk processes encoded by uniform elements of $\mathcal{W}_n$. Thanks to Proposition 20 we can equivalently study coalescent-walk processes encoded by quadrant walks conditioned to start and end at $(0,0)$. We will first deal with the unconditioned case (see Section 3.1.1) and then with the conditioned one (see Section 3.1.2).

3.1 Scaling limits of coalescent-walk processes

We start by defining our continuous limiting object: it is formed by the solutions of the following family of stochastic differential equations (SDEs) indexed by $u \in \mathbb{R}$, driven by a two-dimensional process $\boldsymbol{\mathcal{W}} = (\boldsymbol{\mathcal{X}}, \boldsymbol{\mathcal{Y}})$

$$\begin{cases} d\mathcal{Z}^{(u)}(t) &= \mathbb{1}_{\{\mathcal{Z}^{(u)}(t)>0\}}\, d\boldsymbol{\mathcal{Y}}(t) - \mathbb{1}_{\{\mathcal{Z}^{(u)}(t)\le 0\}}\, d\boldsymbol{\mathcal{X}}(t), \quad t \geq u, \\ \mathcal{Z}^{(u)}(t) &= 0, \quad t \le u. \end{cases} \tag{7}$$

Existence and uniqueness of solutions were already studied in the literature in the case where the driving process $\boldsymbol{\mathcal{W}}$ is a Brownian motion, in particular with the following result.

▶ **Theorem 21** (Theorem 2 of [23], Proposition 2.2 of [9]). *Let I be a (finite or infinite) interval of $\mathbb{R}$ and fix $t_0 \in I$. Let $\mathcal{W} = (\mathcal{X}, \mathcal{Y})$ denote a two-dimensional Brownian motion on I with covariance matrix $\left(\begin{smallmatrix} 1 & \rho \\ \rho & 1 \end{smallmatrix}\right)$ for $\rho \in (-1,1)$. We have path-wise uniqueness (explained in 1 below) and existence (explained in 2 below) of a strong solution for the SDE:*

$$\begin{cases} d\mathcal{Z}(t) &= \mathbb{1}_{\{\mathcal{Z}(t)>0\}}\, d\mathcal{Y}(t) - \mathbb{1}_{\{\mathcal{Z}(t)\leq 0\}}\, d\mathcal{X}(t), \quad t \in I \cap [t_0, +\infty), \\ \mathcal{Z}(t_0) &= 0. \end{cases} \tag{8}$$

Namely, letting $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\in I}, \mathbb{P})$ be a filtered probability space satisfying the usual conditions, and assuming that $(\mathcal{X}, \mathcal{Y})$ is an $(\mathcal{F}_t)_t$-Brownian motion,

1. *if $\mathcal{Z}, \mathcal{Z}^\star$ are two $(\mathcal{F}_t)_t$-adapted continuous processes that verify Equation* (8) *almost surely, then $\mathcal{Z} = \mathcal{Z}^\star$ almost surely.*
2. *There exists an $(\mathcal{F}_t)_t$-adapted continuous process $\mathcal{Z}$ which verifies Equation* (8) *almost surely, and is adapted to the completion of the canonical filtration of $(\mathcal{X}, \mathcal{Y})$.*

3.1.1 The unconditioned scaling limit result

Let us now work on the completed canonical filtered probability space of a Brownian motion $\mathcal{W} = (\mathcal{X}, \mathcal{Y})$ with covariance $\begin{pmatrix} 1 & -1/2 \\ -1/2 & 1 \end{pmatrix}$. For $u \in \mathbb{R}$, let $\mathcal{Z}^{(u)}$ be the strong solution of Equation (8) with $I = [u, \infty)$ and $t_0 = u$, provided by Theorem 21. Note that $\mathcal{Z}^{(u)}$ satisfies Equation (8) (only) for almost all ω. For every u, $\mathcal{Z}^{(u)}$ is adapted, and it is simple to see that the map $(\omega, u) \mapsto \mathcal{Z}^{(u)}$ is jointly measurable. By Tonelli's theorem, for almost every ω, $\mathcal{Z}^{(u)}$ is a solution for almost every u.

▶ Remark 22. For fixed u, $\mathcal{Z}^{(u)}$ is a Brownian motion on $[u, \infty)$. Note however that the coupling of $\mathcal{Z}^{(u)}$ for different values of u is highly non trivial.

▶ Remark 23. Given ω (even restricted to a set of probability one), we cannot say that $(\mathcal{Z}^{(u)})_{u\in\mathbb{R}}$ forms a whole field of solutions to Equation (7), since we cannot guarantee that the SDE holds for all u simultaneously. Similarly, it is expected that there exists exceptional u where uniqueness fails.

Now, let $\bar{\boldsymbol{W}} = (\bar{\boldsymbol{X}}, \bar{\boldsymbol{Y}}) = (\bar{\boldsymbol{X}}_k, \bar{\boldsymbol{Y}}_k)_{k\in\mathbb{Z}}$ be the random plane walk defined below Equation (2), and $\bar{\boldsymbol{Z}} = \mathrm{WC}(\bar{\boldsymbol{W}})$ be the corresponding coalescent-walk process. We define rescaled versions: for all $n \geq 1, u \in \mathbb{R}$, let $\bar{\mathcal{W}}_n : \mathbb{R} \to \mathbb{R}^2$ and $\bar{\mathcal{Z}}_n^{(u)} : \mathbb{R} \to \mathbb{R}$ be the continuous functions defined by linearly interpolating the following points:

$$\bar{\mathcal{W}}_n\left(\frac{k}{n}\right) = \frac{1}{\sqrt{2n}}\bar{\boldsymbol{W}}_k, \quad k \in \mathbb{Z}, \qquad \bar{\mathcal{Z}}_n^{(u)}\left(\frac{k}{n}\right) = \frac{1}{\sqrt{2n}}\bar{\boldsymbol{Z}}_k^{(\lfloor nu \rfloor)}, \quad u \in \mathbb{R}, k \in \mathbb{Z}. \tag{9}$$

Our most important technical result is the following theorem (whose proof is postponed to Appendix A).

▶ **Theorem 24.** *Let $u_1 < \ldots < u_k$. We have the following joint convergence in $(\mathcal{C}(\mathbb{R}, \mathbb{R}))^{k+2}$:*

$$\left(\bar{\mathcal{W}}_n, \bar{\mathcal{Z}}_n^{(u_1)}, \ldots, \bar{\mathcal{Z}}_n^{(u_k)}\right) \xrightarrow[n\to\infty]{d} \left(\mathcal{W}, \mathcal{Z}^{(u_1)}, \ldots, \mathcal{Z}^{(u_k)}\right). \tag{10}$$

3.1.2 The conditioned scaling limit result

As a standard application of [12, Theorem 4], the scaling limit of the random walk $\bar{\mathcal{W}}_n$ conditioned on starting at the origin at time 0 and ending at the origin at time $n+1$ is $\mathcal{W}_e = (\mathcal{X}_e, \mathcal{Y}_e)$, the Brownian excursion in the non-negative quadrant of covariance $\left(\begin{smallmatrix} 1 & -1/2 \\ -1/2 & 1 \end{smallmatrix}\right)$. Let us denote by $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{0\leq t\leq 1}, \mathbb{P}_{\text{exc}})$ the completed canonical probability space of $\mathcal{W}_e$, and work from now on in that space.

It makes sense that the scaling limit of the coalescent-walk process in this conditioned setting should be the solution of Equation (7) driven by $\mathcal{W}_e$, for which we have to show existence and uniqueness. First, let us remark that since Brownian excursions are semimartingales, stochastic integrals are still well-defined. We skip the rather abstract proof of the following, which relies on absolute continuity between Brownian excursion and Brownian motion:

▶ **Theorem 25.** *Denote $\mathcal{F}_t^{(u)} = \sigma(\mathcal{W}_e(s) - \mathcal{W}_e(u), u \leq s \leq t)$ completed by the $\mathbb{P}_{\text{exc}}$-negligible sets of Ω. There is a jointly measurable map $(\omega, u) \mapsto \mathcal{Z}_e^{(u)}$ such that for all u, $\mathcal{Z}_e^{(u)}$ is $(\mathcal{F}_t^{(u)})_t$-adapted, and almost surely, for almost every u, $\mathcal{Z}_e^{(u)}$ solves Equation (7) driven by $\mathcal{W}_e$. Moreover, for $u \in (0,1)$, if $\mathcal{Z}^\star$ is another $(\mathcal{F}_t^{(u)})_t$-adapted solution of Equation (7) driven by $\mathcal{W}_e$ started at time u, then $\mathcal{Z}^\star = \mathcal{Z}_e^{(u)}$ almost surely.*

From the above result and the discrete absolutely continuity arguments of [10, 12], we can deduce the following analogous result of Theorem 24 (whose proof is omitted). We use the same notation as in Equation (9), and state the result for uniform random times for later convenience.

▶ **Theorem 26.** *Let $\boldsymbol{u}_1 < \ldots < \boldsymbol{u}_k$ be k sorted independent continuous uniform random variables on $[0,1]$, independent from all other random variables. We have the following convergence in $(\mathcal{C}([0,1],\mathbb{R}))^{k+2}$:*

$$\left(\bar{\mathcal{W}}_n, \bar{\mathcal{Z}}_n^{(\boldsymbol{u}_1)}, \ldots, \bar{\mathcal{Z}}_n^{(\boldsymbol{u}_k)} \middle| (\bar{\boldsymbol{W}}_t)_{0\leq t\leq n+1} \in \mathfrak{W}_{n+2}^{A,\text{exc}}\right) \xrightarrow[n\to\infty]{d} \left(\mathcal{W}_e, \mathcal{Z}_e^{(\boldsymbol{u}_1)}, \ldots, \mathcal{Z}_e^{(\boldsymbol{u}_k)}\right).$$

3.2 The construction of the limiting object

We introduce the limiting *coalescent Baxter permuton.* We place ourselves in the probability space defined above, where $\mathcal{W}_e = (\mathcal{X}_e, \mathcal{Y}_e)$ is a Brownian excursion of correlation $-1/2$ conditioned to stay in the non-negative quadrant. Let $\mathcal{Z}_e = \{\mathcal{Z}_e^{(u)}\}_{u\in[0,1]}$ be the family of processes given by Theorem 25, which almost surely solves Equation (7) driven by $\mathcal{W}_e$ for almost every u. From the continuous coalescent-walk process $\mathcal{Z}_e$ we build a binary relation $\leq_{\mathcal{Z}_e}$ on $[0,1]$ defined as in Equation (6). Clearly, $(\omega, x, y) \mapsto \mathbb{1}_{x\leq_{\mathcal{Z}_e} y}$ is measurable, and we have the following property whose proof, which relies on path-wise uniqueness, is skipped.

▶ **Proposition 27.** *The relation $\leq_{\mathcal{Z}_e}$ is a total order on $[0,1] \setminus \boldsymbol{A}$, where $\boldsymbol{A}$ is a random set of zero Lebesgue measure.*

We then define the following random function (note that $(\omega, t) \mapsto \varphi_{\mathcal{Z}_e}(t)$ is measurable):

$$\begin{aligned} \varphi_{\mathcal{Z}_e}(t) &\coloneqq \operatorname{Leb}\left(\{x \in [0,1] | x \leq_{\mathcal{Z}_e} t\}\right) \\ &= \operatorname{Leb}\left(\{x \in [0,t) | \mathcal{Z}_e^{(x)}(t) < 0\} \cup \{x \in [t,1] | \mathcal{Z}_e^{(t)}(x) \geq 0\}\right), \end{aligned}$$

where here $\operatorname{Leb}(\cdot)$ denotes the one-dimensional Lebesgue measure. We define the *coalescent Baxter permuton* as the push-forward of the Lebesgue measure via the map $(\operatorname{Id}, \varphi_{\mathcal{Z}_e})$, i.e.

$$\boldsymbol{\mu}_B(\cdot) = \mu_{\mathcal{Z}_e}(\cdot) \coloneqq (\operatorname{Id}, \varphi_{\mathcal{Z}_e})_* \operatorname{Leb}(\cdot) = \operatorname{Leb}\left(\{t \in [0,1] | (t, \varphi_{\mathcal{Z}_e}(t)) \in \cdot \,\}\right).$$

▶ **Observation 28.** *We try to give an intuition behind the definition of $\boldsymbol{\mu}_B$. Recall that given a coalescent-walk process $Z = \{Z^{(t)}\}_{t\in[n]} \in \mathcal{C}$, we can associate to it the corresponding Baxter permutation $\sigma = \mathrm{CP}(Z)$ and the total order $\leq_Z$ on $[n]$. The permutation σ satisfies the following property: for every $i \in [n]$, $\sigma(i) = |\{j \in [n] | j \leq_Z i\}|$. The function $\varphi_{\mathfrak{Z}_e}$ is a continuous analogue of the permutation σ, when we consider the continuous coalescent-walk process $\mathfrak{Z}_e$ instead of a discrete one, and $\mu_{\mathfrak{Z}_e}$ is the associated permuton.*

The following result is proved as [20, Proposition 3.1], relying on Proposition 27.

▶ **Proposition 29.** *Almost surely, $\mu_{\mathfrak{Z}_e}$ is a permuton.*

The final proof of Theorem 5, i.e. the convergence of uniform Baxter permutations to $\boldsymbol{\mu}_B$, can be found in Appendix B. We give here a short sketch. The proof is based on the analysis of pattern extraction from uniform Baxter permutations. Proposition 17 relates the probability of extracting a specific pattern to the probability that some trajectories of the corresponding coalescent-walk process have given signs at given times. Then, by Theorem 26, the latter converges to the analogue probability for the limiting continuous coalescent-walk process.

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A The proof of Theorem 24

Recall that $\bar{\boldsymbol{W}} = (\bar{\boldsymbol{X}}, \bar{\boldsymbol{Y}}) = (\bar{\boldsymbol{X}}_k, \bar{\boldsymbol{Y}}_k)_{k\in\mathbb{Z}}$ is the random plane walk defined below Equation (2), and $\bar{\boldsymbol{Z}} = \mathrm{WC}(\bar{\boldsymbol{W}})$ is the corresponding coalescent-walk process. We need the following result whose proof is left to the complete version of this extended abstract.

▶ **Proposition 30.** *For every $u \in \mathbb{Z}$, $\bar{\boldsymbol{Z}}^{(u)}$ has the distribution of a random walk with the same step distribution as $\bar{\boldsymbol{Y}}$ (which is the same as that of $-\bar{\boldsymbol{X}}$).*

▶ Remark 31. Recall that the increments of a walk of a coalescent-walk process are not always equal to one of the increments of the corresponding walk (see for instance Equation (5)). The statement of Proposition 30 is a sort of "miracle" of the geometric distribution.

Proof of Theorem 24. The first step in the proof is to establish convergence of the components of the vector on the left-hand side of Theorem 24. By a classical invariance principle, we get that $\bar{\mathcal{W}}_n = (\bar{\mathcal{X}}_n, \bar{\mathcal{Y}}_n)$ converges to $\mathcal{W} = (\mathcal{X}, \mathcal{Y})$ in distribution. Using Proposition 30, and applying again the invariance principle, we get that $(\bar{\mathcal{Z}}_n^{(u)}(u+t))_{t\geq 0}$, converges to a one-dimensional Brownian motion. This gives the marginal convergence thanks to Remark 22.

The second step in the proof is to establish joint convergence. Marginal convergence gives joint tightness, so that by Prokhorov's theorem, to show convergence, one only needs to identify the distribution of all joint subsequential limits. Assume that along a subsequence, we have

$$\left(\bar{\mathcal{W}}_n, \bar{\mathcal{Z}}_n^{(u_1)}, \dots, \bar{\mathcal{Z}}_n^{(u_k)}\right) \xrightarrow[n\to\infty]{d} \left(\mathcal{W}, \tilde{\mathcal{Z}}_1, \dots, \tilde{\mathcal{Z}}_k\right).$$

Using Skorokhod's theorem, we may define all involved variables on the same probability space and assume that the convergence is almost sure. The joint distribution of the right-hand-side is unknown for now, but we will show that for every $1 \leq i \leq k$, $\tilde{\mathcal{Z}}_i = \mathcal{Z}^{(u_i)}$ a.s., which would complete the proof. Recall that $\mathcal{Z}^{(u_i)}$ is the strong solution of Equation (8), started at time u_i and driven by $\mathcal{W} = (\mathcal{X}, \mathcal{Y})$, which exists thanks to Theorem 21. Let us now fix i and abbreviate $u = u_i$, $\tilde{\mathcal{Z}} = \tilde{\mathcal{Z}}_i$. Our goal is to show that $\tilde{\mathcal{Z}}$ also verifies Equation (8) and apply path-wise uniqueness.

Let $\mathcal{F}_t = \sigma(\boldsymbol{\mathcal{W}}(s), \tilde{\boldsymbol{\mathcal{Z}}}(s), s \le t)$. This gives a filtration for which $\boldsymbol{\mathcal{W}}$ and $\tilde{\boldsymbol{\mathcal{Z}}}$ are adapted. We will show that $\boldsymbol{\mathcal{W}}$ is an $(\mathcal{F}_t)_t$-Brownian motion, that is for $t \in \mathbb{R}, s \ge 0$, $(\boldsymbol{\mathcal{W}}(t+s) - \boldsymbol{\mathcal{W}}(t)) \perp\!\!\!\perp \mathcal{F}_t$. For fixed n, by definition of a random walk, $\bar{\boldsymbol{\mathcal{W}}}_n(t+s) - \bar{\boldsymbol{\mathcal{W}}}_n(t)$ is independent from $\sigma(\bar{\boldsymbol{W}}_k, k \le \lfloor nt \rfloor)$. Therefore, by the definition given in Equation (5),

$$\left(\bar{\boldsymbol{\mathcal{W}}}_n(t+s) - \bar{\boldsymbol{\mathcal{W}}}_n(t)\right) \perp\!\!\!\perp \left(\bar{\boldsymbol{\mathcal{W}}}_n(r), \bar{\boldsymbol{\mathcal{Z}}}_n^{(u)}(r)\right)_{r \le n^{-1}\lfloor nt \rfloor}. \tag{11}$$

By convergence, we obtain that $\boldsymbol{\mathcal{W}}(t+s) - \boldsymbol{\mathcal{W}}(t)$ is independent from $\left(\boldsymbol{\mathcal{W}}(r), \tilde{\boldsymbol{\mathcal{Z}}}(r)\right)_{r \le t}$, completing the claim that $\boldsymbol{\mathcal{W}}$ is an $(\mathcal{F}_t)_t$-Brownian motion.

Now fix a rational $\varepsilon > 0$ and a rational $t > u$ such that $\tilde{\boldsymbol{\mathcal{Z}}}(t) > \varepsilon$. There is $\delta > 0$ so that $\tilde{\boldsymbol{\mathcal{Z}}} > \varepsilon/2$ on $[t-\delta, t+\delta]$. By almost sure convergence, there is N_0 such that for $n \ge N_0$, $\bar{\boldsymbol{\mathcal{Z}}}_n^{(u)} > \varepsilon/4$ on $[t-\delta, t+\delta]$. On this interval, outside of the event

$$\{\sup_{1 \le i \le n} |\bar{\boldsymbol{\mathcal{Y}}}_i - \bar{\boldsymbol{\mathcal{Y}}}_{i-1}| \ge \sqrt{2n}\varepsilon/4\},$$

$\bar{\boldsymbol{\mathcal{Z}}}_n^{(u)} - \bar{\boldsymbol{\mathcal{Y}}}_n$ is constant by construction of the coalescent-walk process. As a result (the probability of the bad event is bounded by $Ce^{-c\sqrt{n}}$), the limit $\tilde{\boldsymbol{\mathcal{Z}}} - \boldsymbol{\mathcal{Y}}$ is constant too almost surely. We have shown that almost surely $\tilde{\boldsymbol{\mathcal{Z}}} - \boldsymbol{\mathcal{Y}}$ is locally constant on $\{t : \tilde{\boldsymbol{\mathcal{Z}}}(t) > \varepsilon\}$. This translates into the following equality:

$$\int_u^t \mathbb{1}_{\{\tilde{\boldsymbol{\mathcal{Z}}}(r) > \varepsilon\}} \, d\tilde{\boldsymbol{\mathcal{Z}}}(r) = \int_u^t \mathbb{1}_{\{\tilde{\boldsymbol{\mathcal{Z}}}(r) > \varepsilon\}} \, d\boldsymbol{\mathcal{Y}}(r).$$

The stochastic integrals are well-defined: on the left-hand side by considering the canonical filtration of $\tilde{\boldsymbol{\mathcal{Z}}}$, on the right-hand-side by considering $(\mathcal{F}_t)_t$. The same can be done for negative values, leading to

$$\int_u^t \mathbb{1}_{\{|\tilde{\boldsymbol{\mathcal{Z}}}(r)| > \varepsilon\}} \, d\tilde{\boldsymbol{\mathcal{Z}}}(r) = \int_u^t \mathbb{1}_{\{\tilde{\boldsymbol{\mathcal{Z}}}(r) > \varepsilon\}} \, d\boldsymbol{\mathcal{Y}}(r) - \int_u^t \mathbb{1}_{\{\tilde{\boldsymbol{\mathcal{Z}}}(r) < -\varepsilon\}} \, d\boldsymbol{\mathcal{X}}(r).$$

By stochastic dominated convergence theorem [24, Thm. IV.2.12], one can take the limit as $\varepsilon \to 0$, and obtain

$$\int_u^t \mathbb{1}_{\{\tilde{\boldsymbol{\mathcal{Z}}}(r) \neq 0\}} \, d\tilde{\boldsymbol{\mathcal{Z}}}(r) = \int_u^t \mathbb{1}_{\{\tilde{\boldsymbol{\mathcal{Z}}}(r) > 0\}} \, d\boldsymbol{\mathcal{Y}}(r) - \int_u^t \mathbb{1}_{\{\tilde{\boldsymbol{\mathcal{Z}}}(r) < 0\}} \, d\boldsymbol{\mathcal{X}}(r).$$

Thanks to the fact that $\tilde{\boldsymbol{\mathcal{Z}}}$ is Brownian, $\int_u^t \mathbb{1}_{\{\tilde{\boldsymbol{\mathcal{Z}}}(r)=0\}} \, d\tilde{\boldsymbol{\mathcal{Z}}}(r) = 0$, so that the left-hand side equals $\tilde{\boldsymbol{\mathcal{Z}}}(t)$. As a result $\tilde{\boldsymbol{\mathcal{Z}}}$ verifies Equation (8) and we can apply path-wise uniqueness (Theorem 21) to complete the proof. ◀

B The proof of Theorem 5

Recall that permuton convergence has been defined in Definition 4. We present one its characterizations (which comes from [1, Theorem 2.5]), expressed in terms of random induced patterns. For $n \in \mathbb{Z}_{>0}$, we denote by $\mathfrak{S}_n$ the set of permutations of size n. Let $1 \le k \le n$, $\sigma \in \mathfrak{S}_n$ and $I = \{i_1, \dots i_k\}$ with $1 \le i_1 < \dots < i_k \le n$. The pattern in σ induced by I is the only permutation $\pi \in \mathfrak{S}_k$ such that the k values $\sigma(i_1), \dots, \sigma(i_k)$ are order isomorphic to $\pi(1), \dots, \pi(k)$. In this case, we write $\mathrm{pat}_I(\sigma) = \pi$.

We also define permutations induced by k points in the square $[0,1]^2$. Take a sequence of k points $(X,Y)=((x_1,y_1),\dots,(x_k,y_k))$ in $[0,1]^2$ in general position, i.e. with distinguished x and y coordinates. We denote by $(x_{(1)},y_{(1)}),\dots,(x_{(k)},y_{(k)})$ the x-reordering of (X,Y), i.e. the unique reordering of the sequence $((x_1,y_1),\dots,(x_k,y_k))$ such that $x_{(1)}<\dots<x_{(k)}$. Then the values $(y_{(1)},\dots,y_{(k)})$ are in the same relative order as the values of a unique permutation, that we call the *permutation induced by* (X,Y).

▶ **Proposition 32.** *Let $\boldsymbol{\sigma}_n$ be a random permutation of size n, and $\boldsymbol{I}_n^k=\{\boldsymbol{i}_n^1,\dots,\boldsymbol{i}_n^k\}$ be a uniform k-element subset of $[n]$, independent of $\boldsymbol{\sigma}_n$. Let $\boldsymbol{\mu}$ be a random permuton, and denote $\mathrm{Perm}_k(\boldsymbol{\mu})$ the unique permutation*[9] *induced by k independent points in $[0,1]^2$ with common distribution $\boldsymbol{\mu}$ conditionally*[10] *on $\boldsymbol{\mu}$. Then*

$$\mu_{\boldsymbol{\sigma}_n}\xrightarrow{d}\boldsymbol{\mu}\iff\forall k\in\mathbb{Z}_{>0},\ \forall\pi\in\mathfrak{S}_k,\quad\mathbb{P}(\mathrm{pat}_{\boldsymbol{I}_n^k}(\boldsymbol{\sigma}_n)=\pi)\to\mathbb{P}(\mathrm{Perm}_k(\boldsymbol{\mu})=\pi).$$

We can now prove Theorem 5. First we state a consequence of the fact that $\mu_{\mathfrak{Z}_e}$ is a permuton and that $\mathfrak{Z}_e^{(s)}(t)$ are continuous random variables, which allows us to get rid of equalities:

▶ **Lemma 33.** *Almost surely, for almost every $s<t\in[0,1]$, $\mathfrak{Z}_e^{(s)}(t)\neq 0$. Then $\mathfrak{Z}_e^{(s)}(t)>0$ implies $\varphi_{\mathfrak{Z}_e}(s)<\varphi_{\mathfrak{Z}_e}(t)$, and $\mathfrak{Z}_e^{(s)}(t)<0$ implies $\varphi_{\mathfrak{Z}_e}(s)>\varphi_{\mathfrak{Z}_e}(t)$.*

Proof of Theorem 5. We reuse here the notation of Theorem 26. In particular $\bar{\boldsymbol{W}}$ is a ν-random walk and $\bar{\boldsymbol{Z}}=\mathrm{WC}(\bar{\boldsymbol{W}})$ is the associated coalescent-walk process. Let $\boldsymbol{\sigma}_n=\mathrm{CP}(\bar{\boldsymbol{Z}}|_{[n]})$. Let $\mathcal{E}_n$ denote the event $\{(\bar{\boldsymbol{W}}_t)_{0\le t\le n+1}\in\mathfrak{W}_{n+2}^{A,\mathrm{exc}}\}$. By Proposition 20 and the fact that the mapping $\mathrm{CP}\circ\mathrm{WC}$ is a size-preserving bijection, conditioned on $\mathcal{E}_n$, $\boldsymbol{\sigma}_n$ is a uniform Baxter permutation.

Fix $k\ge 1$ and $\pi\in\mathfrak{S}_k$. For $n\ge k$, let $\boldsymbol{I}_n=\{\boldsymbol{i}_n^1,\dots,\boldsymbol{i}_n^k\}$ be a uniform k-element subset of $[n]$, independent of $\boldsymbol{\sigma}_n$. In view of Proposition 32, to complete the proof, we will show that

$$\mathbb{P}(\mathrm{pat}_{\boldsymbol{I}_n}(\boldsymbol{\sigma}_n)=\pi\mid\mathcal{E}_n)\xrightarrow[n\to\infty]{}\mathbb{P}(\mathrm{Perm}_k(\mu_{\mathfrak{Z}_e})=\pi).$$

Thanks to Proposition 17, we have

$$\mathbb{P}(\mathrm{pat}_{\boldsymbol{I}_n}(\boldsymbol{\sigma}_n)=\pi\mid\mathcal{E}_n)=\mathbb{P}\left(\forall_{1\le\ell<s\le k},\ \bar{\boldsymbol{Z}}_{\boldsymbol{i}_n^s}^{(\boldsymbol{i}_n^\ell)}\ge 0\iff\pi(\ell)>\pi(s)\mid\mathcal{E}_n\right).$$

Let $(\boldsymbol{u}_1,\dots,\boldsymbol{u}_k)$ be the sorted vector of k independent uniform continuous random variables in $[0,1]$. For every $n\ge 1$, one can couple $\boldsymbol{I}_n$ and $(\boldsymbol{u}_1,\dots,\boldsymbol{u}_k)$ so that $\boldsymbol{i}_n^j=\lfloor n\boldsymbol{u}_j\rfloor$ for every $1\le j\le k$, with an error of probability $O(1/n)$. As a result,

$$\begin{aligned}\mathbb{P}(\mathrm{pat}_{\boldsymbol{I}_n}(\boldsymbol{\sigma}_n)=\pi\mid\mathcal{E}_n)&=\mathbb{P}\left(\forall_{1\le\ell<s\le k},\ (2n)^{-1/2}\bar{\boldsymbol{Z}}_{\boldsymbol{u}_s}^{(\boldsymbol{u}_\ell)}\ge 0\iff\pi(\ell)>\pi(s)\mid\mathcal{E}_n\right)+O(1/n)\\&\xrightarrow[n\to\infty]{}\mathbb{P}\left(\forall_{1\le\ell<s\le k},\ \mathfrak{Z}_e^{(\boldsymbol{u}_\ell)}(\boldsymbol{u}_s)\ge 0\iff\pi(\ell)>\pi(s)\right)\\&=\mathbb{P}\left(\forall_{1\le\ell<s\le k},\begin{cases}\pi(\ell)>\pi(s)\implies\varphi_{\mathfrak{Z}_e}(\boldsymbol{u}_\ell)>\varphi_{\mathfrak{Z}_e}(\boldsymbol{u}_s)\\\pi(\ell)<\pi(s)\implies\varphi_{\mathfrak{Z}_e}(\boldsymbol{u}_\ell)<\varphi_{\mathfrak{Z}_e}(\boldsymbol{u}_s)\end{cases}\right),\end{aligned}\tag{12}$$

where for the limit we used the convergence in distribution of Theorem 26 together with the Portmanteau theorem. Additionally, Lemma 33 is used both to take care of the boundary effect in the Portmanteau theorem, and to do the rewriting in the last line.

In order to finish the proof, it is enough to check that the probability on the right-hand side of Equation (12) equals $\mathbb{P}(\mathrm{Perm}_k(\mu_{\mathfrak{Z}_e})=\pi)$. This is clear since by definition of Perm_k and $\mu_{\mathfrak{Z}_e}$, $\mathrm{Perm}_k(\mu_{\mathfrak{Z}_e})$ is the permutation induced by $\big((\boldsymbol{u}_1,\varphi_{\mathfrak{Z}_e}(\boldsymbol{u}_1)),\dots,(\boldsymbol{u}_k,\varphi_{\mathfrak{Z}_e}(\boldsymbol{u}_k))\big)$. ◀

[9] Note that if μ is a permuton, then it has uniform marginals and so the x and y coordinates of k points sampled according to μ are a.s. distinct.

[10] This is possible by considering the new probability space described in [1, Section 2.1].

C Simulations of large Baxter permutations

The simulations for Baxter permutations presented in the first page of this extended abstract have been obtained in the following way:

1. first, we have sampled a uniform random walk of size $n+2$ in the non-negative quadrant starting at $(0,0)$ and ending at $(0,0)$ with increments distribution given by Equation (2). This has been done using a "rejection algorithm": it is enough to sample a walk W starting at $(0,0)$ with increments distribution given by Equation (2), up to the first time it leaves the non-negative quadrant. Then one has to check if the last step inside the non-negative quadrant is at the origin $(0,0)$. When this is the case (otherwise we resample a new walk), the part of the walk W inside the non-negative quadrant, denoted $\tilde{W}$, is a uniform walk of size $|\tilde{W}|$ in the non-negative quadrant starting at $(0,0)$ and ending at $(0,0)$ with increments distribution given by Equation (2).
2. Removing the first and the last step of $\tilde{W}$, thanks to Proposition 20, we obtained a uniform random walk in $\mathcal{W}_n$.
3. Finally, applying the mapping $\mathrm{CP} \circ \mathrm{WC}$ to the walk given by the previous step, we obtained a uniform Baxter permutation of size n (thanks to Theorem 1).

Note that our algorithm gives a uniform Baxter permutation of random size.

More Models of Walks Avoiding a Quadrant

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Abstract

We continue the enumeration of plane lattice paths avoiding the negative quadrant initiated by the first author in [1]. We solve in detail a new case, the king walks, where all 8 nearest neighbour steps are allowed. As in the two cases solved in [1], the associated generating function is proved to differ from a simple, explicit D-finite series (related to the enumeration of walks confined to the first quadrant) by an algebraic one. The principle of the approach is the same as in [1], but challenging theoretical and computational difficulties arise as we now handle algebraic series of larger degree.

We also explain why we expect the observed algebraicity phenomenon to persist for 4 more models, for which the quadrant problem is solvable using the reflection principle.

2012 ACM Subject Classification Theory of computation → Random walks and Markov chains; Mathematics of computing → Enumeration; Mathematics of computing → Generating functions; Mathematics of computing → Computations on polynomials

Keywords and phrases Enumerative combinatorics, lattice paths, non-convex cones, algebraic series, D-finite series

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.8

Funding *Michael Wallner*: Supported by the Erwin Schrödinger Fellowship of the Austrian Science Fund (FWF): J 4162-N35.

Acknowledgements We thank our referees for their careful reading.

1 Introduction

In this paper we continue the enumeration of plane lattice paths confined to non-convex cones initiated by the first author in [1]. Therein the two most natural models of walks confined to the three-quadrant cone $\mathcal{C} := \{(i, j) : i \geq 0 \text{ or } j \geq 0\}$ were studied: walks with steps $\{\rightarrow, \uparrow, \leftarrow, \downarrow\}$, and those with steps $\{\nearrow, \nwarrow, \swarrow, \searrow\}$. In both cases, the generating function that counts walks starting at the origin was proved to differ (additively) from a simple explicit D-finite series by an algebraic one. The tools essentially involved power series manipulations, coefficient extractions, and polynomial elimination.

Later, Raschel and Trotignon gave in [13] sophisticated integral expressions for 8 models, which imply that 3 additional models ($\{\nearrow, \leftarrow, \downarrow\}$, $\{\rightarrow, \uparrow, \swarrow\}$, and $\{\rightarrow, \nearrow, \uparrow, \leftarrow, \swarrow, \downarrow\}$) are D-finite. Their results use an analytic approach inspired by earlier work on probabilistic and enumerative aspects of quadrant walks [5, 12].

In this paper we first extend the results of [1] to the so-called *king walks*, which take their steps from $\{\rightarrow, \nearrow, \uparrow, \nwarrow, \leftarrow, \swarrow, \downarrow, \searrow\}$. We show that the *algebraicity phenomenon* of [1] persists: if $Q(x, y; t)$ (resp. $C(x, y; t)$) counts walks starting from the origin that are confined

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 8; pp. 8:1–8:14
Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

to the non-negative quadrant $\mathcal{Q} := \{(i,j) : i \geq 0 \text{ and } j \geq 0\}$ (resp. to the cone $\mathcal{C}$) by the length (variable t) and the coordinates of the endpoint (variables x, y), then $C(x,y;t)$ differs from the series

$$\frac{1}{3}\left(Q(x,y;t) - Q(1/x,y;t)/x^2 - Q(x,1/y;t)/y^2\right)$$

by an algebraic series, as detailed in our main theorem below. Moreover, we expect a similar property to hold (with variations on the above linear combination of the series Q) for the 7 step sets of Figure 1, related to reflection groups, and for which the quadrant problem can be solved using the reflection principle [7]. However, we also expect the effective solution of these models to be extremely challenging in computational terms, mostly, because the relevant algebraic series have very large degree. This is illustrated by our main theorem below. There, and in the sequel, we use the shorthand $\bar{x} = 1/x$, $\bar{y} = 1/y$, and omit in the notation the dependencies on t, writing for instance $Q(x,y)$ instead of $Q(x,y;t)$.

▶ **Theorem 1.** *Take the step set $\{-1,0,1\}^2 \setminus \{(0,0)\}$ and let $Q(x,y)$ be the generating function of lattice walks starting from $(0,0)$ that are confined to the first quadrant $\mathcal{Q}$ (this series is D-finite and given in [3]). Then, the generating function of walks starting from $(0,0)$, confined to $\mathcal{C}$, and ending in the first quadrant (resp. at a negative abscissa) is*

$$\frac{1}{3}Q(x,y) + P(x,y), \qquad (\textit{resp.} -\frac{\bar{x}^2}{3}Q(\bar{x},y) + \bar{x}M(\bar{x},y)), \tag{1}$$

where $P(x,y)$ and $M(x,y)$ are algebraic of degree 216 over $\mathbb{Q}(x,y,t)$. Of course, the generating function of walks ending at a negative ordinate follows, using the x/y-symmetry.

The series P is expressed in terms of M by:

$$P(x,y) = \bar{x}\big(M(x,y) - M(0,y)\big) + \bar{y}\big(M(y,x) - M(0,x)\big), \tag{2}$$

and M is defined by the following equation:

$$\begin{aligned} K(x,y)\,(2M(x,y) - M(0,y)) = \frac{2x}{3} - 2t\bar{y}(x+1+\bar{x})M(x,0) + t\bar{y}(y+1+\bar{y})M(y,0) \\ + t(x-\bar{x})(y+1+\bar{y})M(0,y) - t\left(1+\bar{y}^2 - 2\bar{x}\bar{y}\right)M(0,0) - t\bar{y}M_x(0,0), \end{aligned} \tag{3}$$

where $K(x,y) = 1 - t(x + xy + y + \bar{x}y + \bar{x} + \bar{x}\bar{y} + \bar{y} + x\bar{y})$. The specializations $M(x,0)$ and $M(0,y)$ are algebraic each of degree 72 over $\mathbb{Q}(x,t)$ and $\mathbb{Q}(y,t)$, respectively, and $M(0,0)$ and $M_x(0,0)$ have degree 24 over $\mathbb{Q}(t)$.

We have moreover a complete algebraic description of all the series needed to reconstruct $P(x,y)$ and $M(x,y)$ from (2) and (3), namely the univariate series $M(0,0)$ and $M_x(0,0)$, and the bivariate series $M(x,0)$ and $M(0,y)$. In particular, both univariate series lie in the extension of $\mathbb{Q}(t)$ (the field of rational functions in t) generated in 3 steps as follows: first, $u = t + t^2 + \mathcal{O}(t^3)$ is the only series in t satisfying

$$(1-3u)^3(1+u)t^2 + (1+18u^2-27u^4)t - u = 0, \tag{4}$$

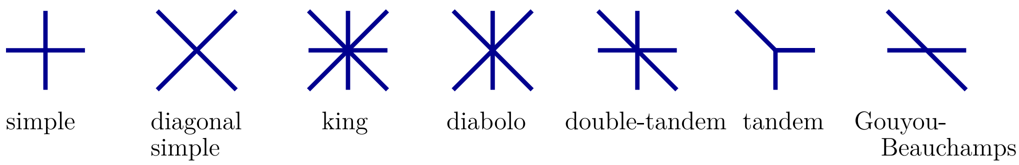

Figure 1 The seven step sets to which the strategy of this paper should apply. The first two are solved in [1], the third one in this paper.

then $v = t + 3t^2 + \mathcal{O}(t^3)$ is the only series with constant term zero satisfying

$$(1 + 3v - v^3)u - v(v^2 + v + 1) = 0, \tag{5}$$

and finally

$$w = \sqrt{1 + 4v - 4v^3 - 4v^4} = 1 + 2t + 4t^2 + \mathcal{O}(t^3). \tag{6}$$

Schematically, $\mathbb{Q}(t) \overset{4}{\hookrightarrow} \mathbb{Q}(t,u) \overset{3}{\hookrightarrow} \mathbb{Q}(t,v) \overset{2}{\hookrightarrow} \mathbb{Q}(t,w)$. Of particular interest is the series $M(0,0)$: by (1), this is also the series $C_{-1,0}$ that counts by the length walks in $\mathcal{C}$ ending at $(-1,0)$. It is algebraic, as conjectured in [13], and given by

$$M(0,0) = C_{-1,0} = \frac{1}{2t}\left(\frac{w(1+2v)}{1+4v-2v^3} - 1\right) = t + 2t^2 + 17t^3 + 80t^4 + 536t^5 + \mathcal{O}(t^6). \tag{7}$$

Due to the lack of space, the extensions of $\mathbb{Q}(x,t)$ generated by $M(x,0)$ and $M(0,x)$ will only be described in the long version of this paper.

Once the series $C(x,y)$ is determined, we can derive detailed asymptotic results, which refine general results of Denisov and Wachtel [4] and Mustapha [11] (who only obtain the following estimates up to a multiplicative factor).

▶ **Corollary 2.** *The number $c_{0,0}(n)$ of n-step king walks confined to $\mathcal{C}$ and ending at the origin, and the number $c(n)$ of walks of $\mathcal{C}$ ending anywhere satisfy for $n \to \infty$:*

$$c_{0,0}(n) \sim \left(\frac{2^{29}K}{3^7}\right)^{1/3} \frac{\Gamma(2/3)}{\pi} \frac{8^n}{n^{5/3}},$$

$$c(n) \sim \left(\frac{2^{32}K}{3^7}\right)^{1/6} \frac{1}{\Gamma(2/3)} \frac{8^n}{n^{1/3}},$$

where K is the unique real root of $101^6K^3 - 601275603K^2 + 92811K - 1$.

Outline of the paper

We begin in Section 2 with a general discussion on models of walks with small steps confined to the cone $\mathcal{C}$, and on the related functional equations. The main part of the paper, Section 3, is devoted to the solution of the king model. We sketch in the final Section 4 what should be the starting point for the 4 rightmost models of Figure 1.

Some definitions and notation

Let $\mathbb{A}$ be a commutative ring and x an indeterminate. We denote by $\mathbb{A}[x]$ (resp. $\mathbb{A}[[x]]$) the ring of polynomials (resp. formal power series) in x with coefficients in $\mathbb{A}$. If $\mathbb{A}$ is a field, then $\mathbb{A}(x)$ denotes the field of rational functions in x, and $\mathbb{A}((x))$ the field of Laurent series in x, that is, series of the form $\sum_{n\ge n_0} a_n x^n$, with $n_0 \in \mathbb{Z}$ and $a_n \in \mathbb{A}$. The coefficient of x^n in a series $F(x)$ is denoted by $[x^n]F(x)$.

This notation is generalized to polynomials, fractions, and series in several indeterminates. If $F(x, x_1, \ldots, x_d)$ is a series in the x_i's whose coefficients are Laurent series in x, say

$$F(x, x_1, \ldots, x_d) = \sum_{i_1,\ldots,i_d} x_1^{i_1} \cdots x_d^{i_d} \sum_{n \ge n_0(i_1,\ldots,i_d)} a(n, i_1, \ldots, i_d) x^n,$$

then the *non-negative part of F in x* is the following formal power series in $x, x_1, \ldots, x_d$:

$$[x^{\ge 0}]F(x, x_1, \ldots, x_d) = \sum_{i_1,\ldots,i_d} x_1^{i_1} \cdots x_d^{i_d} \sum_{n\ge 0} a(n, i_1, \ldots, i_d) x^n.$$

We define similarly the negative part of F, its positive part, and so on. We denote with bars the reciprocals of variables: that is, $\bar{x} = 1/x$, so that $\mathbb{A}[x, \bar{x}]$ is the ring of Laurent polynomials in x with coefficients in $\mathbb{A}$.

If $\mathbb{A}$ is a field, a power series $F(x) \in \mathbb{A}[[x]]$ is *algebraic* (over $\mathbb{A}(x)$) if it satisfies a non-trivial polynomial equation $P(x, F(x)) = 0$ with coefficients in $\mathbb{A}$. It is *differentially finite* (or *D-finite*) if it satisfies a non-trivial linear differential equation with coefficients in $\mathbb{A}(x)$. For multivariate series, D-finiteness requires the existence of a differential equation *in each variable*. We refer to [8, 9] for general results on D-finite series.

As mentioned above, we usually omit the dependency in t of our series. For a series $F(x, y; t) \in \mathbb{Q}[x, \bar{x}, y, \bar{y}][[t]]$ and two integers i and j, we denote by $F_{i,j}$ the coefficient of $x^i y^j$ in $F(x, y; t)$. This is a series in $\mathbb{Q}[[t]]$.

2 Enumeration in the three-quarter plane

We fix a subset $\mathcal{S}$ of $\{-1, 0, 1\}^2 \setminus \{(0, 0)\}$ and we want to count walks with steps in $\mathcal{S}$ that start from the origin $(0, 0)$ of $\mathbb{Z}^2$ and remain in the cone $\mathcal{C} := \{(x, y) : x \geq 0 \text{ or } y \geq 0\}$. By this, we mean that not only must every vertex of the walk lie in $\mathcal{C}$, but also every edge: a walk containing a step from $(-1, 0)$ to $(0, -1)$ (or vice versa) is not considered as lying in $\mathcal{C}$. We often say for short that our walks *avoid the negative quadrant*. The *step polynomial* of $\mathcal{S}$ is defined by

$$S(x, y) = \sum_{(i,j)\in\mathcal{S}} x^i y^j = \bar{y}H_-(x) + H_0(x) + yH_+(x) = \bar{x}V_-(y) + V_0(y) + xV_+(y),$$

for some Laurent polynomials H_-, H_0, H_+ and V_-, V_0, V_+ (of degree at most 1 and valuation at least -1) recording horizontal and vertical displacements, respectively. We denote by $C(x, y; t) \equiv C(x, y)$ the generating function of walks confined to $\mathcal{C}$, where the variable t records the length of the walk, and x and y the coordinates of its endpoints:

$$C(x, y) = \sum_{(i,j)\in\mathcal{C}} \sum_{n\geq 0} c_{i,j}(n) x^i y^j t^n = \sum_{(i,j)\in\mathcal{C}} x^i y^j C_{i,j}(t). \tag{8}$$

Here, $c_{i,j}(n)$ is the number of walks of length n that go from $(0, 0)$ to (i, j) and that are confined to $\mathcal{C}$.

2.1 Interesting step sets

As in the quadrant case [3], we can decrease the number of step sets that are worth being considered (*a priori*, there are 2^8 of them) thanks to a few simple observations:

- Since the cone $\mathcal{C}$ (as well as the quarter plane $\mathcal{Q}$) is x/y-symmetric, the models defined by $\mathcal{S}$ and by its mirror image $\overline{\mathcal{S}} := \{(j, i) : (i, j) \in \mathcal{S}\}$ are equivalent; the associated generating functions are related by $\overline{C}(x, y) = C(y, x)$.
- If all steps of $\mathcal{S}$ are contained in the right half-plane $\{(x, y) : x \geq 0\}$, then *all* walks with steps in $\mathcal{S}$ lie in $\mathcal{C}$, and the series $C(x, y) = 1/(1 - tS(x, y))$ is simply rational. The series $Q(x, y)$ is known to be algebraic in this case [6].
- If all steps of $\mathcal{S}$ are contained in the left half-plane $\{(x, y) : x \leq 0\}$, then confining a walk to $\mathcal{C}$ is equivalent to confining it to the upper half-plane: the associated generating function is then algebraic, and so is $Q(x, y)$.
- If all steps of $\mathcal{S}$ lie (weakly) above the first diagonal $(x = y)$, then confining a walk to $\mathcal{C}$ is again equivalent to confining it to the upper half-plane: the associated generating function is then algebraic, and so is $Q(x, y)$.

- Finally, if all steps of $\mathcal{S}$ lie (weakly) above the second diagonal ($x+y=0$), then all walks with steps in $\mathcal{S}$ lie in $\mathcal{C}$, and $C(x,y)=1/(1-tS(x,y))$ is simply rational. In this case however, the series $Q(x,y)$ is not at all trivial [3,10]. Such step sets are sometimes called *singular* in the framework of quadrant walks.

Symmetric statements allow us to discard step sets that lie in the upper half-plane $\mathbb{Z}\times\mathbb{N}$, in the lower half-plane $\mathbb{Z}\times(-\mathbb{N})$, or weakly below the x/y diagonal.

In conclusion, one finds that there are exactly 51 essentially distinct models of walks avoiding the negative quadrant that are worth studying: the 56 models considered for quadrant walks (see Tables 1–4 in [3]) except the 5 singular models for which all steps of $\mathcal{S}$ lie weakly above the diagonal $x+y=0$.

2.2 A functional equation

Constructing walks confined to $\mathcal{C}$ step by step gives the following functional equation:

$$C(x,y)=1+tS(x,y)C(x,y)-t\bar{y}H_-(x)C_{-,0}(\bar{x})-t\bar{x}V_-(y)C_{0,-}(\bar{y})-t\bar{x}\bar{y}C_{0,0}\mathbb{1}_{(-1,-1)\in\mathcal{S}},$$

where the series $C_{-,0}(\bar{x})$ and $C_{0,-}(\bar{y})$ count walks ending on the horizontal and vertical boundaries of $\mathcal{C}$ (but not at $(0,0)$):

$$C_{-,0}(\bar{x})=\sum_{\substack{i<0\\ n\geq 0}}c_{i,0}(n)x^it^n\in\bar{x}\mathbb{Q}[\bar{x}][[t]],$$
$$C_{0,-}(\bar{y})=\sum_{\substack{j<0\\ n\geq 0}}c_{0,j}(n)y^jt^n\in\bar{y}\mathbb{Q}[\bar{y}][[t]].$$

On the right-hand side of the above functional equation, the term 1 accounts for the empty walk, the next term describes the extension of a walk in $\mathcal{C}$ by one step of $\mathcal{S}$, and each of the other three terms correspond to a "bad" move, either starting from the negative x-axis, or from the negative y-axis, or from $(0,0)$. Equivalently,

$$K(x,y)C(x,y)=1-t\bar{y}H_-(x)C_{-,0}(\bar{x})-t\bar{x}V_-(y)C_{0,-}(\bar{y})-t\bar{x}\bar{y}C_{0,0}\mathbb{1}_{(-1,-1)\in\mathcal{S}}, \tag{9}$$

where $K(x,y):=1-tS(x,y)$ is the *kernel* of the equation.

The case of walks confined to the first (non-negative) quadrant $\mathcal{Q}$ has been much studied in the past 15 years. The associated generating function $Q(x,y)\equiv Q(x,y;t)\in\mathbb{Q}[x,y][[t]]$ is defined similarly to (8) and satisfies a similarly looking equation:

$$K(x,y)Q(x,y)=1-t\bar{y}H_-(x)Q_{-,0}(x)-t\bar{x}V_-(y)Q_{0,-}(y)+t\bar{x}\bar{y}Q_{0,0}\mathbb{1}_{(-1,-1)\in\mathcal{S}},$$

where now

$$Q_{-,0}(x)=\sum_{\substack{i\geq 0\\ n\geq 0}}q_{i,0}(n)x^it^n=Q(x,0)\in\mathbb{Q}[x][[t]],$$
$$Q_{0,-}(y)=\sum_{\substack{j\geq 0\\ n\geq 0}}q_{0,j}(n)y^jt^n=Q(0,y)\in\mathbb{Q}[y][[t]].$$

3 The king walks

In this section we focus on the case where the 8 steps of $\{-1,0,1\}^2\setminus\{(0,0)\}$ are allowed. That is,

$$S(x,y)=(\bar{x}+1+x)(\bar{y}+1+y)-1=x+xy+y+\bar{x}y+\bar{x}+\bar{x}\bar{y}+\bar{y}+x\bar{y}.$$

The functional equation (9) specializes to

$$K(x,y)C(x,y) = 1 - t\bar{y}(x+1+\bar{x})C_-(\bar{x}) - t\bar{x}(y+1+\bar{y})C_-(\bar{y}) - t\bar{x}\bar{y}C_{0,0}, \tag{10}$$

where we have denoted $C_-(\bar{x}) = C_{-,0}(\bar{x}) = C_{0,-}(\bar{x})$ (by symmetry). Equivalently,

$$xyK(x,y)C(x,y) = xy - t(x^2+x+1)C_-(\bar{x}) - t(y^2+y+1)C_-(\bar{y}) - tC_{0,0}. \tag{11}$$

The generating function $Q(x,y)$ of quadrant walks satisfies

$$xyK(x,y)Q(x,y) = xy - t(x^2+x+1)Q(x,0) - t(y^2+y+1)Q(0,y) + tQ_{0,0}. \tag{12}$$

3.1 Reduction to an equation with orbit sum zero

A key object in the study of walks confined to the first quadrant is a certain group of birational transformations that depends on the step set. For king walks, it is generated by $(x,y) \mapsto (\bar{x},y)$ and $(x,y) \mapsto (x,\bar{y})$. As in [1], the similarities between the equations for C and Q, combined with the structure of this group, lead us to define a new series $A(x,y)$ by

$$C(x,y) = A(x,y) + \frac{1}{3}\left(Q(x,y) - \bar{x}^2Q(\bar{x},y) - \bar{y}^2Q(x,\bar{y})\right). \tag{13}$$

Then the combination of (11) and (12) gives

$$xyK(x,y)A(x,y) = \frac{2xy+\bar{x}y+x\bar{y}}{3} - t(x^2+x+1)A_-(\bar{x}) - t(y^2+y+1)A_-(\bar{y}) - tA_{0,0},$$

and it follows from this equation that $xyA(x,y)$ has *orbit sum* zero. By this, we mean:

$$xyA(x,y) - \bar{x}yA(\bar{x},y) + \bar{x}\bar{y}A(\bar{x},\bar{y}) - x\bar{y}A(x,\bar{y}) = 0. \tag{14}$$

Theorem 1 states that $A(x,y)$ is algebraic. In Section 4 we define an analogous series A for all models of Figure 1 which we expect to be systematically algebraic.

The proof of Theorem 1 starts as in the case of the simple and diagonal walks in [1]. The first objective, achieved in Section 3.5, is to derive an equation that involves a single bivariate series, essentially $A_-(x)$ (and no trivariate series). In principle, the "generalized quadratic method" of [2] then solves it routinely. But in practise, the king model turns out to be much more difficult to solve than the other two, and raises serious computational difficulties. In what follows, we focus on the points of the derivation that differ from [1]. We have performed all computations with the computer algebra system MAPLE. The corresponding sessions will be available on the authors' webpages with the long version of the paper.

3.2 Reduction to a quadrant-like problem

We separate in $A(x,y)$ the contributions of the three quadrants, again using the x/y-symmetry of the step set:

$$A(x,y) = P(x,y) + \bar{x}M(\bar{x},y) + \bar{y}M(\bar{y},x),$$

where $P(x,y)$ and $M(x,y)$ lie in $\mathbb{Q}[x,y][[t]]$. Note that this identity defines P and M uniquely in terms of A. Replacing A by this expression, and extracting the positive part in x and y from the orbit equation (14) relates the series P and M by

$$xyP(x,y) = y\left(M(x,y) - M(0,y)\right) + x\left(M(y,x) - M(0,x)\right),$$

which is exactly the same as [1, Eq. (22)], and as Eq. (2) in Theorem 1. We then follow the lines of proof of [1, Sec. 2.3] to obtain the functional equation (3) for M.

3.3 An equation between $M(0,x)$, $M(0,\bar{x})$, and $M(x,0)$

Next we will cancel the kernel K. As a polynomial in y, the kernel admits only one root that is a formal power series in t:

$$Y(x) = \frac{1-t(x+\bar{x}) - \sqrt{(1-t(x+\bar{x}))^2 - 4t^2(x+1+\bar{x})^2}}{2t(x+1+\bar{x})} = (x+1+\bar{x})t + \mathcal{O}(t^2).$$

Note that $Y(x) = Y(\bar{x})$. We specialize (3) to the pairs $(x, Y(x)), (\bar{x}, Y(x)), (Y(x), x)$, and $(Y(x), \bar{x})$ (the left-hand side vanishes for each specialization since $K(x,y) = K(y,x)$), and eliminate $M(0,Y)$, $M(Y,0)$, and $M(\bar{x},0)$ from the four resulting equations. We obtain:

$$\begin{aligned}(x+1+\bar{x})\left(Y(x) - \frac{1}{Y(x)}\right)&(xM(0,x) - 2\bar{x}M(0,\bar{x})) + 3(x+1+\bar{x})M(x,0) \\ &- \frac{2\bar{x}Y(x)}{t} + 3M_{1,0} + (2Y(x) - x - \bar{x})M_{0,0} = 0.\end{aligned} \tag{15}$$

3.4 An equation between $M(0,x)$ and $M(0,\bar{x})$

Let us denote the discriminant occurring in $Y(x)$ by

$$\Delta(x) := (1-t(x+\bar{x}))^2 - 4t^2(x+1+\bar{x})^2 = (1-t(3(x+\bar{x})+2))(1+t(x+\bar{x}+2)) \tag{16}$$

and introduce the notation

$$\begin{aligned}R(x) &:= t^2M(x,0) = \frac{xt^2}{3} + \left(1 + \frac{x^2}{3}\right)t^3 + \mathcal{O}(t^4), \\ S(x) &:= txM(0,x) = x(1+x)t^2 + 2x(1+x+x^2)t^3 + \mathcal{O}(t^4).\end{aligned} \tag{17}$$

Then (15) reads

$$\begin{aligned}\sqrt{\Delta(x)}\left(S(x) - 2S(\bar{x}) + \frac{R(0) - t\bar{x}}{t(x+1+\bar{x})}\right) &= 3(x+1+\bar{x})R(x) + 3R'(0) \\ &+ \frac{1-t(x+\bar{x})(x+2+\bar{x})}{t(x+1+\bar{x})}R(0) - \frac{1-t(x+\bar{x})}{1+x+x^2}.\end{aligned} \tag{18}$$

Next, we square this equation and extract the negative part in x. The series $R(x)$ (mostly) disappears as it involves only non-negative powers of x. This gives an expression for the negative part of $\Delta(x)S(x)S(\bar{x})$. Using the symmetry of $\Delta(x)$ in x and $\bar{x}$, we then reconstruct an expression of $\Delta(x)S(x)S(\bar{x})$ that does not involve $R(x)$, as in [1, Sec. 2.5].

During these calculations, we have to extract the negative and non-negative parts in series of the form $F(x)/(1+x+\bar{x})^m$, where $F(x)$ is a series in t with coefficients in $\mathbb{Q}[x,\bar{x}]$. Upon performing a partial fraction expansion, and separating in F the negative and non-negative parts, we see that the key question is how to extract and express the non-negative part in series of the form $F(\bar{x})/(1-\zeta_i x)^m$, where $F(x) \in \mathbb{C}[x][[t]]$ and

$$\zeta_1 := -\frac{1}{2} + \frac{i\sqrt{3}}{2} \quad \text{and} \quad \zeta_2 := -\frac{1}{2} - \frac{i\sqrt{3}}{2}$$

are the primitive cubic roots of unity. A simple calculation establishes the following lemma.

▶ **Lemma 3** (Non-negative part at pole ρ). *Let $F(x) \in \mathbb{C}[x][[t]]$ and $\rho \in \mathbb{C}$. Then,*

$$\begin{aligned}[x^{\geq 0}]\frac{F(\bar{x})}{1-\rho x} &= \frac{F(\rho)}{1-\rho x}, \\ [x^{\geq 0}]\frac{F(\bar{x})}{(1-\rho x)^2} &= \frac{F(\rho)}{(1-\rho x)^2} + \frac{\rho F'(\rho)}{1-\rho x}.\end{aligned}$$

One outcome of the extraction procedure is the following identity:

$$S(\zeta_1) = S(\zeta_2) = -\frac{R(0) + 3R'(0)}{1+t} = -t^2 - 11t^4 - 30t^5 + \mathcal{O}(t^6). \tag{19}$$

Using these results, we finally arrive at an equation relating $S(x)$ and $S(\bar{x})$:

$$\begin{aligned} \Delta(x) \left(S(x)^2 + S(\bar{x})^2 - S(x)S(\bar{x}) + \frac{S(x)(xt - R(0)) + \bar{x}S(\bar{x})(\bar{x}t - R(0))}{t(x+1+\bar{x})} \right) = \\ (1+t)S(\zeta_1) \left(2(x+1+\bar{x})R(0) - \frac{(1 - t(x+\bar{x}))(t(x+\bar{x}) - 2R(0))}{t(x+1+\bar{x})} \right) \\ +(1+4t)(x+\bar{x})R(0) - (t^2 + tR(0) + R(0)^2)(x^2+\bar{x}^2) + \Delta_0, \end{aligned} \tag{20}$$

where Δ_0 is the coefficient of x^0 in $\Delta(x)S(x)S(\bar{x})$.

3.5 An equation for $M(0, x)$ only

Equation (20) is almost ready for a positive part extraction, except for the mixed term $S(x)S(\bar{x})$. To eliminate it, we multiply (20) by $S(x) + S(\bar{x}) + \frac{x+\bar{x}-2R(0)/t}{x+1+\bar{x}}$. Then we are able to extract the non-negative terms in x. Hereby we repeatedly apply Lemma 3. Additionally, we use $R(0) = tS'(0)$ and (19). Furthermore, we work with the real and imaginary parts of $\zeta_1 S'(\zeta_1)$ and $\zeta_2 S'(\zeta_2)$. More precisely, we define

$$(1+t)^2\zeta_1 S'(\zeta_1) = B_1 + i\sqrt{3}B_2,$$
$$(1+t)^2\zeta_2 S'(\zeta_2) = B_1 - i\sqrt{3}B_2.$$

(Note that B_1 and B_2 here are series in t.) In the end we get a cubic equation in $S(x)$:

$$\mathrm{Pol}(S(x), S'(0), S(\zeta_1), B_1, B_2, t, x) = 0, \tag{21}$$

where the polynomial $\mathrm{Pol}(x_0, x_1, x_2, x_3, x_4, t, x)$ is given in Appendix A.

3.6 The generalized quadratic method

We now use the results of [2] to obtain a system of four polynomial equations relating the series $S'(0), S(\zeta_1), B_1$, and B_2. Combined with a few initial terms, this system characterizes these four series. Unfortunately, it turned out to be too big for us to solve it completely, be it by bare hand elimination or using Gröbner bases: we did obtain a polynomial equation for $S'(0)$ and $S(\zeta_1)$, but not for the other two series. Instead, we have resorted to a guess-and-check approach, consisting in *guessing* such equations (of degree 12 or 24, depending on the series), and then *checking* that they satisfy the system. This guess-and-check approach is detailed in the next subsection. For the moment, let us explain how the system is obtained.

The approach of [2] instructs us to consider the fractional series X (in t), satisfying

$$\mathrm{Pol}_{x_0}(S(X), S'(0), S(\zeta_1), B_1, B_2, t, X) = 0, \tag{22}$$

where Pol_{x_0} stands for the derivative of Pol with respect to its first variable. The number and first terms of such series X depend only on the first terms of the series $S(x), S'(0), S(\zeta_1), B_1$, and B_2 (see [2, Thm. 2]). We find that 6 such series exist:

$$\begin{aligned}
X_1(t) &= i + 2t^2 + 4t^3 + (36-2i)t^4 + \mathcal{O}(t^5),\\
X_2(t) &= -i + 2t^2 + 4t^3 + (36+2i)t^4 + \mathcal{O}(t^5),\\
X_3(t) &= \sqrt{t} + t + \frac{3}{2}t^{3/2} + 3t^2 + \frac{51}{8}t^{5/2} + 14t^3 + \mathcal{O}(t^{7/2}),\\
X_4(t) &= -\sqrt{t} + t - \frac{3}{2}t^{3/2} + 3t^2 - \frac{51}{8}t^{5/2} + 14t^3 + \mathcal{O}(t^{7/2}),\\
X_5(t) &= i\sqrt{t} - it^{3/2} + 2it^{5/2} + t^3 - 4it^{7/2} + 2t^4 + \mathcal{O}(t^{9/2}),\\
X_6(t) &= -i\sqrt{t} + it^{3/2} - 2it^{5/2} + t^3 + 4it^{7/2} + 2t^4 + \mathcal{O}(t^{9/2}).
\end{aligned}$$

Note that the coefficients of X_1 and X_2 (resp. X_5 and X_6) are conjugates of one another. As discussed in [2], each of these series X also satisfies

$$\mathrm{Pol}_x(S(X), S'(0), S(\zeta_1), B_1, B_2, t, X) = 0, \tag{23}$$

where Pol_x is the derivative with respect to the last variable of Pol, and (of course)

$$\mathrm{Pol}(S(X), S'(0), S(\zeta_1), B_1, B_2, t, X) = 0. \tag{24}$$

Using this, we can easily identify two of the series X_i: indeed, eliminating B_1 and B_2 between the three equations (22), (23), and (24) gives a polynomial equation between $S(X), S'(0), S(\zeta_1), t$, and X, which factors. Remarkably, its simplest non-trivial factor does not involve $S(X)$, nor $S'(0)$ nor $S(\zeta_1)$, and reads

$$X^2 - t(1+X)^2(1+X^2). \tag{25}$$

By looking at the first terms of the X_i's and the other factors, one concludes that the above equation holds for X_3 and X_4, which are thus explicit.

Let $D(x_1, \dots, x_4, t, x)$ be the discriminant of $\mathrm{Pol}(x_0, \dots, x_4, t, x)$ with respect to x_0. According to [2, Thm. 14], each X_i is a *double root* of $D(S'(0), S(\zeta_1), B_1, B_2, t, x)$, seen as a polynomial in x. Hence this polynomial, which involves 4 unknown series $S'(0), S(\zeta_1), B_1, B_2$, has (at least) 6 double roots. This seems more information than we need! In principle, 4 double roots should suffice to give 4 conditions relating the 4 unknown series. However, we shall see that there is some redundancy in the 6 series X_i, which comes from the special form of D.

We first observe that D factors as

$$D(S'(0), S(\zeta_1), B_1, B_2, t, x) = 27x^2(1+x+x^2)^2\Delta(x) D_1(S'(0), S(\zeta_1), B_1, B_2, t, x),$$

where $\Delta(x)$ is defined by (16), and D_1 has degree 24 in x. It is easily checked that none of the X_i's are roots of the prefactors, so they are double roots of D_1. But we observe that D_1 is symmetric in x and $\bar{x}$. More precisely,

$$D_1(S'(0), S(\zeta_1), B_1, B_2, t, x) = x^{12} D_2(S'(0), S(\zeta_1), B_1, B_2, t, x + 1 + \bar{x}),$$

for some polynomial $D_2(x_1, \dots, x_4, t, s) \equiv D_2(s)$ of degree 12 in s. Since each X_i is a double root of D_1, each series $S_i := X_i + 1 + 1/X_i$, for $1 \le i \le 6$, is a double root of D_2. The series S_i, for $2 \le i \le 6$, are easily seen from their first terms to be distinct, but the first terms of S_1 and S_2 suspiciously agree: one suspects (and rightly so), that $X_2 = 1/X_1$, and carefully concludes that D_2 has (at least) 5 double roots in s. Moreover, since X_3 and X_4 satisfy (25), the corresponding series S_3 and S_4 are the roots of $1+t=tS_i^2$, that is, $S_{3,4}=\pm\sqrt{1+1/t}$. The other roots start as follows:

$$S_2 = 1+4t^2+8t^3+\mathcal{O}(t^4), \qquad S_{5,6} = \mp\frac{i}{\sqrt{t}}+1+t^2\pm it^{5/2}+\mathcal{O}(t^3).$$

But this is not the end of the story: indeed, D_2 appears to be almost symmetric in s and $1/s$. More precisely, we observe that

$$D_2(S'(0),S(\zeta_1),B_1,B_2,s) = s^6 D_3\left(S'(0),S(\zeta_1),B_1,B_2,ts+\frac{t+1}{s}\right),$$

for some polynomial $D_3(S'(0),S(\zeta_1),B_1,B_2,t,z)\equiv D_3(z)$ of degree 6 in z. It follows that each series $Z_i := tS_i+(1+t)/S_i$, for $2\le i\le 6$, is a root of $D_3(z)$, and even a double root, unless $tS_i^2=1+t$, which precisely occurs for $i=3,4$. One finds $Z_{3,4}=\pm 2\sqrt{t(1+t)}$,

$$Z_2 = 1+2t-4t^2+\mathcal{O}(t^3), \qquad Z_{5,6} = 2t+2t^3+\mathcal{O}(t^4).$$

Since Z_5 and Z_6 seem indistinguishable, we safely conclude that $D_3(z)$ has two double roots Z_2 and Z_5, and a factor $(z^2-4t(1+t))$. Writing

$$D_3(z) = \sum_{i=0}^{6} d_i z^i,$$

these properties imply, by matching the three monomials of highest degree, that

$$D_3(z) = \frac{\left(z^2-4\,t(1+t)\right)\left(8\,z^2{d_6}^2+4\,zd_5d_6+16\,t^2{d_6}^2+16\,t{d_6}^2+4\,d_4d_6-{d_5}^2\right)^2}{64\,{d_6}^3}.$$

Extracting the coefficients of $z^0,\dots,z^3$ gives 4 polynomial relations between the coefficients d_i, resulting in 4 polynomial relations between the 4 series $S'(0),S(\zeta_1),B_1,B_2$. One easily checks that this system, combined with the first terms of these series, defines them uniquely.

As explained at the beginning of this subsection, we have at the moment only been able to derive from this system polynomial equations (of degree 24) for $S'(0)$ and $S(\zeta_1)$. For the other two, we had to resort to a guess-and-check approach, which we now describe.

3.7 Guess-and-check

Guessing. Returning to the functional equation (10) it is easy to extract a simple recurrence for the polynomials $c_n(x,y)$ that count walks of length n by the position of their endpoint. We implemented this recurrence in the programming language C using modular arithmetic and the Chinese remainder theorem to compute the explicit values of this sequence up to $n=2000$. Then we were able to guess polynomial equations satisfied by $S'(0)$, $S(\zeta_1)$, B_1, and B_2 using the `gfun` package in Maple [14]. Of course, those obtained for $S'(0)$ and $S(\zeta_1)$ coincide with those that we derived from the system of the previous subsection. Details on the corresponding equations are shown below.

Generating function	Degree in GF	Degree in t	Number of terms
$S'(0)$	24	12	323
$S(\zeta_1)$	24	32	823
B_1	12	26	229
B_2	24	60	477

Checking that the guessed series satisfy the system turns out to be much easier once the algebraic structure of these series is elucidated, which we do below[1]. We have not tried a direct check.

The algebraic structure of $S'(0), S(\zeta_1), B_1$, and B_2. We begin with the simplest series, B_1, of (conjectured) degree 12. Let $P(F,t)$ be its guessed monic minimal polynomial. Using the `Subfields` command of MAPLE for several fixed values of t, one conjectures that the extension $\mathbb{Q}(t,B_1)$ possesses a subfield $Q(t,u)$ of degree 4 over $\mathbb{Q}(t)$. MAPLE gives a possible generator u for fixed values of t, but how can we choose u for a generic t? Indeed, the value of u given by MAPLE for fixed t has no reason to be canonical. But the factorisation of $P(F,t)$ over $\mathbb{Q}(t,u)$, of the form $P_3(F)P_9(F)$ (with P_i of degree i), with coefficients in $\mathbb{Q}(t,u)$, *is* canonical. Hence we will compute this factorisation, first for fixed values of t. We proceed as follows: we factor $P(F,t)$ over $\mathbb{Q}(t,B_1)$, and find, for fixed $t=3,\dots,50$, that

$$P(F,t) = (F-B_1)P_2(F,B_1)P_9(F,B_1),$$

where P_2 (resp. P_9) is a monic polynomial of degree 2 (resp. 9) in F. Hence the cubic factor $P_3(F) = F^3 + p_2F^2 + p_1F + p_0$ must be $(F-B_1)P_2(F,B_1)$, and we have just found its coefficients p_i in terms of B_1 (for t fixed). We now compute the minimal polynomial over $\mathbb{Q}$ of each p_i using a resultant or the `evala/Norm` command in MAPLE. If the above factorization persists for all t, as we expect, each p_i should have a minimal polynomial over $\mathbb{Q}(t)$ of degree (at most) 4. Having computed this polynomial for sufficiently many values of t, we reconstruct its generic form by rational reconstruction. We find that all p_i generate the same extension of degree 4 of $\mathbb{Q}(t)$, and we can take any of them as a first candidate for the generator u. We may simplify this generator further to end with the choice (4). Then we factor $P(F,t)$ over $\mathbb{Q}(t,u)$, and check that our guess was correct: the series B_1 is indeed cubic over $\mathbb{Q}(t,u)$. Moreover, it can be written rationally in terms of t and the series v given by (5).

Finally, we factor the guessed minimal polynomials of $S'(0)$, $S(\zeta_1)$, and B_2 over $\mathbb{Q}(t,v)$, and find that these three series all belong to the same quadratic extension of $\mathbb{Q}(t,v)$, generated by the series w given by (6). In particular,

$$S'(0) = \frac{1}{2}\left(\frac{w(1+2v)}{1+4v-2v^3} - 1\right),$$

which coincides with (7), given the Definition (17) of $S(x)$.

Now that we have guessed rational expressions of $S'(0)$, $S(\zeta_1)$, B_1, and B_2 in terms of t, v, and w, the 4 equations obtained in Section 3.6 are readily checked to hold, using the minimal polynomials of v and w.

3.8 Back to $S(x)$ and $R(x)$

For $S(x)$ we start with Equation (21), with all one-variable series replaced by their expressions in terms of t, v, and w. We eliminate w and v using resultants to arrive at an equation of degree 72 over $\mathbb{Q}(t,x)$ for $S(x) = txM(0,x)$.

[1] For this section, we have greatly benefited from the help of Mark van Hoeij (`https://www.math.fsu.edu/~hoeij/`), who explained us how to find subextensions of $\mathbb{Q}(t,B_1)$, and "simple" series in these extensions.

We can simplify (21) by working with the depressed equation, i.e., removing the quadratic term by a suitable change of variable. Indeed, defining $T(x)$ by

$$S(x) = T(x) + \frac{3xS'(0) - 2x^2 - 1}{3(x^2 + x + 1)},$$

we find that $T(x)$ satisfies a cubic equation with no quadratic term, involving t and v but not w. That is, $T(x)$ has degree 36 over $\mathbb{Q}(t, x)$, instead of 72 for $S(x)$.

Introducing $T(x)$ also helps understanding the algebraic structure of $R(x)$. Returning to (18), we recall that $R(0) = tS'(0)$ and use (19) to express $R'(0)$ in terms of t, v, and w. The left-hand side simply reads $\sqrt{\Delta(x)}(T(x) - 2T(\bar{x}))$, and is found to be an element of $w\mathbb{Q}(t, x, T(x))$. In the end, $R(x)$ has degree 72 and belongs to the same extension of $\mathbb{Q}(t, x)$ as $S(x)$. This ends the proof of our main result, Theorem 1.

4 More models

For each of the 7 step sets $\mathcal{S}$ of Figure 1, we are able to define a series $A(x, y)$ that

- satisfies the same equation as $C(x, y)$ (see (9)), but with a different constant term,
- satisfies an *orbit sum* identity similar to (14).

Explaining where this series comes from would require us to introduce the group associated to a step set. For the sake of conciseness, we simply define $A(x, y)$ without further justification.

For the first four step sets $\mathcal{S}$ of Figure 1, the series $A(x, y)$ is defined by (13) (with $Q(x, y)$ counting quadrant walks with steps in $\mathcal{S}$) as we have seen. For the next two step sets,

$$C(x, y) = A(x, y) + \frac{1}{5}\left(Q(x, y) - \bar{x}^2 yQ(\bar{x}y, y) + \bar{x}^3 Q(\bar{x}y, \bar{x}) + \bar{y}^3 Q(\bar{y}, x\bar{y}) - x\bar{y}^2 Q(x, x\bar{y})\right).$$

Finally, for the seventh one,

$$\begin{aligned} C(x, y) = A(x, y) + \frac{1}{7}\big(&Q(x, y) - \bar{x}^2 yQ(\bar{x}y, y) + \bar{x}^4 yQ(\bar{x}y, \bar{x}^2 y) \\ &- \bar{x}^4 Q(\bar{x}, \bar{x}^2 y) - \bar{y}^3 Q(x\bar{y}, \bar{y}) + x^2\bar{y}^3 Q(x\bar{y}, x^2\bar{y}) - x^2\bar{y}^2 Q(x, x^2\bar{y})\big). \end{aligned}$$

In all cases, the series $A(x, y)$ satisfies the following variant of (9):

$$K(x, y)A(x, y) = P_0(x, y) - t\bar{y}H_-(x)A_{-,0}(\bar{x}) - t\bar{x}V_-(y)A_{0,-}(\bar{y}) - t\bar{x}\bar{y}A_{0,0}\mathbb{1}_{(-1,-1)\in\mathcal{S}},$$

where $K(x, y) = 1 - tS(x, y)$ as before, and $P_0(x, y)$ is a Laurent polynomial. This equation is easily obtained by combining the equations for $C(x, y)$ and $Q(x, y)$.

Finally, the vanishing orbit sum, which is (14) for the first four models, reads

$$xyA(x, y) - \bar{x}y^2 A(\bar{x}y, y) + \bar{x}^2 yA(\bar{x}y, \bar{x}) - \bar{x}\bar{y}A(\bar{y}, \bar{x}) + x\bar{y}^2 A(\bar{y}, x\bar{y}) - x^2\bar{y}A(x, x\bar{y}) = 0$$

for the next two, and

$$\begin{aligned} &xyA(x, y) - \bar{x}y^2 A(\bar{x}y, y) + \bar{x}^3 y^2 A(\bar{x}y, \bar{x}^2 y) - \bar{x}^3 yA(\bar{x}, \bar{x}^2 y) \\ &\qquad + \bar{x}\bar{y}A(\bar{x}, \bar{y}) - x\bar{y}^2 A(x\bar{y}, \bar{y}) + x^3\bar{y}^2 A(x\bar{y}, x^2\bar{y}) - x^3\bar{y}A(x, x^2\bar{y}) = 0 \end{aligned}$$

for the last one. We conjecture that the series $A(x, y)$ is systematically algebraic (this is now proved for the first three models). To support this conjecture, we have tried to guess (using the `gfun` package [14] in MAPLE), for the 4 models for which it is still open, a polynomial equation for the series $A_{-1,0}$, which, in all cases, coincides with the generating function $C_{-1,0}$

of walks ending at $(-1,0)$ (for the second model we consider $A_{-2,0}$ instead, since $A_{-1,0}=0$ due to the periodicity of the model). This series has degree 4 (resp. 8, 24) in the three solved cases. We could not guess anything for the 4th model (using the counting sequence for such walks up to length $n=4000$), but we discovered equations of degree 24 for each of the next three.

We believe that it would be worth exploring if the guiding principles of the present paper apply to these 4 other models. In all cases, we expect to face a *system* of quadrant-like equations rather than a single one. We plan to investigate at least some of these models.

To conclude, we recall that the 4 small step models that are algebraic for the quadrant problem are conjectured to be algebraic for the three-quadrant cone as well [1, Fig. 5]. In this case, the series $A(x,y)$ simply coincides with $C(x,y)$, as the orbit sum of $xyC(x,y)$ vanishes.

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A Final polynomial equation for $S(x)$ in the king model

The polynomial Pol involved in the cubic Equation (21) defining $S(x)$ is:

$$
\begin{aligned}
&\mathrm{Pol}(x_0, x_1, x_2, x_3, x_4, t, x) = \\
&- 3(x^2+x+1)^2(x^2t+2xt+x+t)(3x^2t+2xt-x+3t)\,\boldsymbol{x_0^3} \\
&\quad + 3(x^2+x+1)(x^2t+2xt+x+t)(3x^2t+2xt-x+3t)(3x_1x-2x^2-1)\,\boldsymbol{x_0^2} \\
&\quad + \big[3x^2(x^2+x+1)^2(2x_4x_1+x_4-x_3) - 3x^2(t+1)^2(x^2+x+1)^2x_2^2 \\
&\quad + 6x(t+1)(x^2+x+1)(x^4t+2x^2t+x^2+t)x_1x_2 \\
&\quad + 3x(t+1)(x^2+x+1)(x^4t-x^3t-x^3+x^2t-xt-x+t)x_2 - 3\left(x^8t^2+2x^7t^2\right. \\
&\quad \left.+10x^6t^2+20x^5t^2+4x^5t+25x^4t^2+20x^3t^2-2x^4+4x^3t+10x^2t^2+2xt^2+t^2\right)x_1^2 \\
&\quad - 3\left(x^8t^2-11x^7t^2-x^7t-32x^6t^2-9x^6t-53x^5t^2-6x^5t-55x^4t^2+3x^5-15x^4t\right. \\
&\quad \left.-39x^3t^2-6x^3t-16x^2t^2+x^3-5x^2t-5xt^2-xt+t^2\right)x_1 - 12x^8t^2-30x^7t^2-6x^7t \\
&\quad - 51x^6t^2-60x^5t^2+3x^6-12x^5t-54x^4t^2-36x^3t^2+3x^4-6x^3t-21x^2t^2-6xt^2 \\
&\quad -3t^2\big]\,\boldsymbol{x_0} + x^2(x^2+x+1)\left[(2x_3x^2-6x_4x-2x_3)x_1^2-(x^2+2)x_3+3x_4x^2\right. \\
&\quad \left.+(2x-1)(3x_4x+x_3(x+2))x_1\right] + 3x^3(t+1)^2(x^2+x+1)(x_1-x)x_2^2 \\
&\quad - 3x^2(t+1)x_2(x_1-x)((2(x^2+t(x^2+1)^2))x_1+t(x^4+x^2+1)-(t+1)x(x^2+1)) \\
&\quad + 3xt(x^2+x+1)^2(x_1-x)(t(x^2-x+1)x_1^2+(x^2t-5xt-x+t)x_1+t(x^2-x+1)).
\end{aligned}
$$

Polyharmonic Functions And Random Processes in Cones

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Abstract

We investigate polyharmonic functions associated to Brownian motions and random walks in cones. These are functions which cancel some power of the usual Laplacian in the continuous setting and of the discrete Laplacian in the discrete setting. We show that polyharmonic functions naturally appear while considering asymptotic expansions of the heat kernel in the Brownian case and in lattice walk enumeration problems. We provide a method to construct general polyharmonic functions through Laplace transforms and generating functions in the continuous and discrete cases, respectively. This is done by using a functional equation approach.

2012 ACM Subject Classification Mathematics of computing → Markov processes; Theory of computation → Random walks and Markov chains; Mathematics of computing → Enumeration; Mathematics of computing → Generating functions

Keywords and phrases Brownian motion in cones, Heat kernel, Random walks in cones, Harmonic functions, Polyharmonic functions, Complete asymptotic expansions, Functional equations

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.9

Funding *François Chapon*: F. C. is supported by the grant ANR-18-CE40-0006 MESA funded by the French National Research Agency (ANR).
Éric Fusy: É. F. is supported by the grant ANR-16-CE40-0009-01 GATO funded by the French National Research Agency (ANR).
Kilian Raschel: This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme under the Grant Agreement No. 759702.

Acknowledgements We would like to thank Cédric Lecouvey, Steve Melczer, Pierre Tarrago and Wolfgang Woess for very interesting discussions. This project has started in July 2019, when two authors were invited at the Institute of Mathematical Statistics of Münster University. The institute, and in particular Gerold Alsmeyer, is greatly acknowledged for hospitality. The first author also acknowledges the Institut Denis Poisson for the warm hospitality during his stay at the Université de Tours, where part of this work has been pursued. Finally, we thank the three anonymous referees for useful comments.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 9; pp. 9:1–9:19
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

1 Introduction and motivations

In the continuous setting, polyharmonic functions are functions which cancel some power of the usual Laplacian. More precisely, a function v on some domain K of $\mathbb{R}^d$ satisfying

$$\Delta^p v = 0$$

for some $p \geq 1$, where Δ is the usual Laplacian in $\mathbb{R}^d$, is said to be *polyharmonic* of order p, or *polyharmonic* for short. So polyharmonic functions of order 1 are just harmonic functions. Obviously, a polyharmonic function v_p of order p satisfies $\Delta v_p = v_{p-1}$, where v_{p-1} is polyharmonic of order $p-1$. For example, polynomials are polyharmonic. Harmonic functions have been tremendously investigated and pioneer works on polyharmonic functions go back to the work of Almansi [1]. One can consult for instance the monograph [2] for an introduction to this topic.

In particular, Almansi [1] proved that if the domain K is star-like with respect to the origin, then every polyharmonic function of order p admits a unique decomposition

$$f(x) = \sum_{k=0}^{p-1} |x|^{2k} h_k(x), \tag{1}$$

where each h_k is harmonic on K and $|x|$ is the Euclidean length of x, hence completely characterising continuous polyharmonic functions on such domains.

In comparison with the continuous case, much less is known in the discrete setting, where the Laplacian has to be replaced by a discrete difference operator. Some progress in understanding discrete polyharmonic functions has been made in the last two decades. For instance, one may cite [12], where the authors investigated polyharmonic functions for the Laplacian on trees, and proved a similar result as Almansi's theorem (1) for homogeneous trees. Recent works of Woess and co-authors [18, 21] are generalising this previous work.

Our original motivation to study discrete polyharmonic functions comes from the following framework. Consider a walk in $\mathbb{Z}^d$ with step set $\mathcal{S}$ confined in some cone $K \subset \mathbb{Z}^d$. Denote by $q(x, y; n)$ the number of n-length excursions between x and y staying in the cone K. To simplify, we only consider the case where y is the origin, but all considerations below can be generalised to $y \neq 0$. In various cases [15], the asymptotics of $q(x, 0; n)$ as $n \to \infty$ is known to admit the form

$$q(x, 0; n) \sim v_0(x)\gamma^n n^{-\alpha_0}, \tag{2}$$

where $v_0(x) > 0$ is a function depending only on x, $\gamma \in (0, |\mathcal{S}|]$ is the exponential growth, and α_0 is the critical exponent. It is easy to see that the function $v_0(x)$ in (2) defines a discrete harmonic function. Indeed, plugging (2) into the obvious recursive relation

$$q(x, 0; n+1) = \sum_{s \in \mathcal{S}} q(x+s, 0; n)\mathbf{1}_{\{x+s \in K\}}, \tag{3}$$

dividing by $\gamma^{n+1} n^{-\alpha_0}$ and letting $n \to \infty$, we obtain

$$v_0(x) = \frac{1}{\gamma} \sum_{s \in \mathcal{S}} v_0(x+s)\mathbf{1}_{\{x+s \in K\}}, \tag{4}$$

which proves that, with the assumption that $v_0(x) = 0$ for $x \notin K$, $v_0(x)$ is discrete harmonic for the Laplacian operator

$$Lf(x) = \frac{1}{\gamma} \sum_{s \in \mathcal{S}} f(x+s) - f(x), \tag{5}$$

that is, $Lv_0 = 0$. Denisov and Wachtel [15] go further and show that

- the exponential growth γ is $\min_{\mathbb{R}_+^d} \sum_{(s_1,\ldots,s_d)\in\mathcal{S}} x_1^{s_1}\cdots x_d^{s_d}$, it does not depend on K;
- the critical exponent α_0 equals $1+\sqrt{\lambda_1+(d/2-1)^2}$, where d is the dimension and λ_1 is the principal Dirichlet eigenvalue on some spherical domain constructed from K.

As a leading example, consider the simple random walk in the quarter plane, with step set $\{\leftarrow,\uparrow,\rightarrow,\downarrow\}$. In this case, the number of excursions $q((i,j),0;n)$ is 0 if $m=\frac{n-i-j}{2}$ is not a non-negative integer, and otherwise takes the value

$$q((i,j),0;n)=\frac{(i+1)(j+1)n!(n+2)!}{m!(m+i+j+2)!(m+i+1)!(m+j+1)!},\tag{6}$$

see [9] and our Example 6. The equivalence (2) is then

$$q((i,j),0;n)\sim\frac{4}{\pi}4^n\frac{v_0(i,j)}{n^3},\tag{7}$$

where $v_0(i,j)=(i+1)(j+1)$ is the well-known unique (up to multiplicative constants) harmonic function positive within the quarter plane with Dirichlet boundary conditions. Other examples of such asymptotics may be found for instance in [4, 10, 14].

Our aim in this discrete setting is to study more precise estimates than (2), by considering complete asymptotic expansions of the following form, as $n\to\infty$,

$$q(x,0;n)\sim\gamma^n\sum_{p\geq 0}\frac{v_p(x)}{n^{\alpha_p}}.\tag{8}$$

From such an asymptotic expansion and using similar ideas as in (3), (4) and (5), it is rather easy to prove that the terms v_p are polyharmonic functions, in the sense that a power $L^k v_p$ of the Laplacian operator vanishes. We will provide examples of such asymptotic expansions (at least for the first terms) and of the set of exponents $\{\alpha_p\}_{p\geq 0}$ appearing in (8).

On the other hand, the functional equation approach has proved to be fruitful when studying random walk problems. The reference book on this topic is the monograph [16] by Fayolle, Iasnogorodski and Malyshev. This method has been used in [20] to construct harmonic functions, both in the discrete and continuous settings. Basically, the method consists of drawing from the harmonicity condition a functional equation satisfied by the generating function (in the discrete setting) or by the Laplace transform (in the continuous setting) of a harmonic function. Solving some boundary value problem for these quantities leads, via Cauchy or Laplace inversion, to the sought harmonic function. We will provide an implementation of this method to construct bi-harmonic functions, which can be generalised to polyharmonic functions.

The main features of our results are as follows:

- We shine a light on a new link between discrete polyharmonic functions and complete asymptotic expansions in the enumeration of walks.
- Our approach provides tools to study complete asymptotics expansions as in (8), but does not allow to prove their existence. On the other hand, the powerful approach of Denisov and Wachtel [15] seems restricted to the first term in the asymptotics (2). Indeed, one of the main tools in [15] is a coupling result of random walks by Brownian motion, which only provides an approximation of polynomial order, see [15, Lem. 17].
- We introduce a new class of functional equations (see (21) and (29)), for which the method of Tutte's invariants introduced in [23, 5, 6] proves to be useful.
- In the unweighted planar case, it has been shown [8] that knowing the rationality of the exponent α_0 in (8) was sufficient to decide the non-D-finiteness of the series of excursions. However, for walks with big steps in dimension two or walk models in dimension three,

this information is not enough [7]. As a potential application of our results, we might use arithmetic information on the other exponents α_p to study the algebraic nature, for example the transcendance, of the associated combinatorial series.

This paper is organised as follows. We choose to start with the continuous setting since computations are more enlightening and accessible. In Section 2, we prove that polyharmonic functions naturally arise when performing an asymptotic expansion of the Dirichlet heat kernel in a cone. We next present the functional equation method to construct polyharmonic functions. Our main result here is Theorem 4, where a class of solutions for the Laplace transform of a bi-harmonic function is provided. It shows that the Laplace transform of a bi-harmonic function can be expressed in terms of the Laplace transform of the related harmonic function plus some additional terms. This can be thought of as a Laplace transform version of Almansi's theorem (1). In Section 3, we exhibit the same phenomenon in the random walk setting. Discrete polyharmonic functions appear when considering the asymptotic expansion of coefficients counting walks with fixed endpoints in a domain, and the functional equation approach may be used to construct discrete polyharmonic functions.

These notes are the starting point of a long-term research project on discrete polyharmonic functions in cones. Notice that many ideas and techniques are not specific to cones and would work for many other domains of restriction K.

2 Classical polyharmonic functions and heat kernel expansions

As pointed out in [2, Chap. VI], the connection between the heat kernel and polyharmonic functions is very profound. Here, we deepen this connection by proving an exact asymptotic expansion for the heat kernel in terms of polyharmonic functions. We then implement the functional equation method to construct polyharmonic functions.

2.1 Exact asymptotic expansion for the Brownian semigroup in a cone

Let K be some cone in $\mathbb{R}^d$ and consider the Brownian motion $(B_t)_{t\geq 0}$ killed at the boundary of K. Denote by $p(x,y;t)$ its transition density, that is the density probability function of the transition probability kernel

$$\mathbb{P}_x(B_t \in dy, \tau > t),$$

where τ is the first exit time of K. Recall the well-known fact that $p(x,y;t)$ corresponds to the heat kernel, i.e., the fundamental solution of the heat equation on K with Dirichlet boundary condition, see for instance [3]. Here, we prove that the heat kernel admits a complete asymptotic expansion in terms of polyharmonic functions for the Laplacian.

Denote by Δ the usual Laplacian on $\mathbb{R}^d$. In polar coordinates (r,θ), where r is the radial part and θ the angular part, it writes:

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{d-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_{\mathbb{S}^{d-1}}, \tag{9}$$

where $\Delta_{\mathbb{S}^{d-1}}$ denotes the spherical Laplacian. Let respectively m_j and λ_j be the Dirichlet (normalised) eigenfunctions and eigenvalues for the spherical Laplacian on the generating set $K \cap \mathbb{S}^{d-1}$, that is,

$$\left\{ \begin{array}{rcll} \Delta_{\mathbb{S}^{d-1}} m_j & = & -\lambda_j m_j & \text{in } K\cap\mathbb{S}^{d-1}, \\ m_j & = & 0 & \text{in } \partial(K\cap\mathbb{S}^{d-1}). \end{array} \right. \tag{10}$$

The eigenvalues satisfy $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots$ by [11, Chap. VII]. We introduce, for $j \geq 1$,

$$\beta_j = \sqrt{\lambda_j + (d/2-1)^2} \quad \text{and} \quad b_j = 1 - d/2 + \sqrt{\lambda_j + (d/2-1)^2}. \tag{11}$$

Lemma 1 in [3] gives an explicit expression for the transition density $p(x, y; t)$ of the Brownian motion in K. It states that, for $x, y \in \mathbb{R}^d$ and $t \in \mathbb{R}_+$,

$$p(x, y; t) = \frac{\exp\left(-\frac{\rho^2+r^2}{2t}\right)}{t(\rho r)^{\frac{d}{2}-1}} \sum_{j=1}^{\infty} I_{\beta_j}\left(\frac{\rho r}{t}\right) m_j(\theta) m_j(\eta), \tag{12}$$

where in polar coordinates $x = (\rho, \theta)$ and $y = (r, \eta)$. Here, I_β is the modified Bessel function of the first kind of order β, satisfying the differential equation $I_\beta''(z) + \frac{1}{z} I_\beta'(z) = (1 + \frac{\beta^2}{z^2}) I_\beta(z)$ and admitting the series expansion

$$I_\beta(z) = \sum_{m=0}^{\infty} \frac{1}{m!\Gamma(m+\beta+1)} \left(\frac{z}{2}\right)^{2m+\beta}. \tag{13}$$

The following easy lemma will allow us to define certain polyharmonic functions.

▶ **Lemma 1.** *For any $\mu \geq 0$ and $j \geq 1$, let $f_{\mu,j}$ be defined in spherical coordinates by*

$$f_{\mu,j}(r, \theta) = r^\mu m_j(\theta). \tag{14}$$

Then $f_{\mu,j}$ satisfies

$$\Delta f_{\mu,j} = (\mu^2 + (d-2)\mu - \lambda_j) f_{\mu-2,j}. \tag{15}$$

Proof. The proof is elementary using (9) and (10). ◀

▶ **Corollary 2.** *For any $k \in \mathbb{N}$, the function $f_{b_j+2k,j}$ defined in (14) is k-polyharmonic.*

Proof. It is obvious that $\mu = b_j$ satisfies $\mu^2 + (d-2)\mu - \lambda_j = 0$, see (11), so that $f_{b_j,j}$ is harmonic by (15). An induction based on (15) completes the proof. ◀

Doing an expansion of the heat kernel (12) as $t \to \infty$ and using series expansions of the exponential function and of the Bessel function (13), one immediately obtains:

▶ **Theorem 3.** *The Dirichlet heat kernel $p(x, y; t)$ in K admits the following expansion, as $t \to \infty$, where $f_{b_j+2k,j}$ is defined in (14), and b_j and β_j in (11):*

$$p(x, y; t) \sim$$
$$\sum_{j\geq 1} \sum_{k,m\geq 0} \sum_{n=0}^{k} \frac{1}{t^{1+\beta_j+k+2m}} \frac{(-1)^k \binom{k}{n}}{2^k k! m! \Gamma(m+\beta_j+1)} f_{b_j+2(m+n),j}(\rho, \theta) f_{b_j+2(m+k-n),j}(r, \eta).$$

As such, the above result shows that the transition density of the Brownian motion in K admits, as $t \to \infty$, an asymptotic expansion in descending powers of t and in terms of polyharmonic functions for the Laplacian (see Corollary 2). Moreover, the set of these exponents is (with $\mathbb{N} = \{0, 1, 2, \dots\}$)

$$\bigcup_{j=1}^{\infty} (\beta_j + 1 + \mathbb{N}). \tag{16}$$

Note that, depending on the cone, there might be an overlap between the sets $\beta_j + 1 + \mathbb{N}$. For instance, in the quadrant in dimension 2, one has $\beta_j = 2j$ and the set in (16) reduces to $\{3, 4, 5, \ldots\}$. On the other hand, in dimension 2 in a cone of opening α such that $\pi/\alpha \notin \mathbb{Q}$, there is no overlap between the points in (16).

As a last remark, we note that the same phenomenon appears for the survival probability $\mathbb{P}_x(\tau > t)$. Indeed, thanks to its explicit expression given by [3, Thm 1] (in terms of the confluent hypergeometric function), one can write down an asymptotic expansion of $\mathbb{P}_x(\tau > t)$ in descending powers of t in terms of polyharmonic functions for the Laplacian.

2.2 The functional equation approach

We apply here the functional equation approach in order to construct polyharmonic functions for the 2-dimensional killed Brownian motion in a convex cone. This approach has been previously introduced in [20] to compute harmonic functions, and is an adaptation of the functional equation method of the random walk case. Our main result is Theorem 4, which gives the general form of the Laplace transform of a bi-harmonic function.

Consider the Brownian motion B in the quarter plane $\mathbb{R}_+^2$ (compared to the last section, we use (x, y) for the coordinates of a 2d point) with covariance matrix

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix},$$

with $\sigma_{11}, \sigma_{22} > 0$ and $\det \Sigma = \sigma_{11}\sigma_{22} - \sigma_{12}^2 \geq 0$. Its infinitesimal generator is the operator

$$\mathcal{G}f = \frac{1}{2}\left(\sigma_{11}\frac{\partial^2 f}{\partial x^2} + 2\sigma_{12}\frac{\partial^2 f}{\partial x \partial y} + \sigma_{22}\frac{\partial^2 f}{\partial y^2}\right).$$

Note that through some linear transformation ϕ (see [20, Eq. (5.1)]), one obtains the Brownian motion with identity covariance matrix in the cone $\phi(\mathbb{R}_+^2)$.

The *kernel* associated to the Brownian motion is defined as the quantity

$$\gamma(x, y) = \frac{1}{2}(\sigma_{11}x^2 + 2\sigma_{12}xy + \sigma_{22}y^2),$$

for $(x, y) \in \mathbb{C}^2$. The Laplace transform of a function f, which in the continuous case is the analogous quantity of the notion of generating function, is defined as

$$L(f)(x, y) = \iint_{[0,\infty)^2} f(u, v)e^{-(xu+yv)}dudv,$$

for $(x, y) \in \mathbb{C}^2$ with positive real parts.

Now, let h be a harmonic function associated with the Brownian motion with covariance matrix Σ, that is, h vanishes on the boundary axes of the quadrant and satisfies $\mathcal{G}h = 0$. The functional equation for h takes the following form (see [20, Eq. (A.1)]):

$$\gamma(x, y)L(h)(x, y) = \frac{1}{2}(\sigma_{11}L_1(h)(y) + \sigma_{22}L_2(h)(x)) + L(\mathcal{G}h)(x, y),$$

where we have denoted

$$\begin{cases} L_1(h)(y) & := & L\left(\frac{\partial h}{\partial x}(0, \cdot)\right)(y) & = & \displaystyle\int_0^\infty \frac{\partial h}{\partial x}(0, v)e^{-yv}dv, \\ L_2(h)(x) & := & L\left(\frac{\partial h}{\partial y}(\cdot, 0)\right)(x) & = & \displaystyle\int_0^\infty \frac{\partial h}{\partial y}(u, 0)e^{-xu}du. \end{cases}$$

Using the harmonicity condition $\mathcal{G}h = 0$, the functional equation for h rewrites as

$$\gamma(x,y)L(h)(x,y) = \frac{1}{2}(\sigma_{11}L_1(h)(y) + \sigma_{22}L_2(h)(x)). \tag{17}$$

We recall below the key argument of the method of [20] to solve the functional equation (17), which leads to harmonic functions for the Brownian motion via Laplace inversion. We will subsequently apply a related method to obtain polyharmonic functions.

Consider the two solutions of $\gamma\left(x, Y(x)\right) = 0$, which, since γ is a homogeneous polynomial of degree two, are explicitly given by $Y_\pm(x) = c_\pm x$, with

$$c_\pm = \frac{-\sigma_{12} \pm i\sqrt{\det \Sigma}}{\sigma_{22}}, \tag{18}$$

so that $c_+ = \overline{c_-}$. We write $c_\pm = ce^{\pm i\theta}$, with $c = \sqrt{\frac{\sigma_{11}}{\sigma_{22}}}$ and θ such that $\cos\theta = -\frac{\sigma_{12}}{\sqrt{\sigma_{11}\sigma_{22}}}$.

Denote by $\mathcal{G}_Y$ the domain delimited by the curve $Y_+([0,\infty]) \cup Y_-([0,\infty]) = c_+[0,\infty] \cup c_-[0,\infty]$ and containing the positive axis $[0,\infty]$. Plugging each of the solutions $c_\pm x$ into the functional equation (17), one obtains a *boundary value problem* for $L_1(h)$, which states that:

1. $L_1(h)$ is analytic on $\mathcal{G}_Y$,
2. $L_1(h)$ is continuous on $\overline{\mathcal{G}_Y} \setminus \{0\}$,
3. For all $x \in (0,\infty]$, $L_1(h)$ satisfies the boundary equation $L_1(h)(c_+x) = L_1(h)(c_-x)$.

In order to solve this problem, one introduces the conformal mapping ω from $\mathcal{G}_Y$ onto $\mathbb{C}\setminus\mathbb{R}_-$ defined by $\omega(x) = x^{-\pi/\theta}$. One eventually obtains that a class of solutions is obtained by letting $L_1(h)$ to be of the form

$$L_1(h)(y) = P\left(\frac{1}{y^{\pi/\theta}}\right), \tag{19}$$

for any given polynomial P. The same applies to $L_2(h)$ (by considering the solutions of $\gamma(X(y), y) = 0$), and using the functional equation (17) and the fact that $(c_\pm)^{\pi/\theta} = -c^{\pi/\theta}$, one must have

$$L_2(h)(y) = -\frac{\sigma_{11}}{\sigma_{22}}P\left(-\frac{1}{c^{\pi/\theta}x^{\pi/\theta}}\right),$$

with the same P as in (19). Hence, using again the functional equation (17), we deduce that the Laplace transform of h writes

$$L(h)(x,y) = \frac{1}{2}\sigma_{11}\frac{P\left(\frac{1}{y^{\pi/\theta}}\right) - P\left(-\frac{1}{c^{\pi/\theta}x^{\pi/\theta}}\right)}{\gamma(x,y)}. \tag{20}$$

In particular, taking P to be a polynomial of degree 1, one gets

$$L(h)(x,y) = \frac{\sigma_{22}\frac{\mu_2}{x^{\pi/\theta}} + \sigma_{11}\frac{\mu_1}{y^{\pi/\theta}}}{\gamma(x,y)},$$

where the constants are related by $\mu_2 = \mu_1(\frac{\sigma_{22}}{\sigma_{11}})^{1-\pi/2\theta}$. Taking the inverse Laplace transform, one should recover the unique positive harmonic function (written in polar coordinates (ρ,η))

$$h(x,y) = \rho^{\frac{\pi}{\theta}}\sin\left(\frac{\pi}{\theta}\eta\right).$$

Suppose now that v is bi-harmonic and satisfies $\mathcal{G}v = h$, where h is harmonic. The functional equation for v now reads

$$\gamma(x,y)L(v)(x,y) = \frac{1}{2}(\sigma_{11}L_1(v)(y) + \sigma_{22}L_2(v)(x)) + L(h)(x,y). \tag{21}$$

By considering the roots of the kernel γ and using the same method as above, we obtain

$$\frac{1}{2}\sigma_{11}L_1(v)(c_+x) - \frac{1}{2}\sigma_{11}L_1(v)(c_-x) = L(h)(x,c_-x) - L(h)(x,c_+x). \tag{22}$$

We now have an *a priori* non-homogeneous boundary value problem for v, that we can in fact transform into an homogeneous one, thanks to the (already known) explicit form of $L(h)$. The key remark to this task is that $(c_+x)^{\pi/\theta} = (c_-x)^{\pi/\theta} = -(cx)^{\pi/\theta}$. Rewriting (20) as

$$L(h)(x,y) = \frac{\sigma_{11}}{\sigma_{22}} \frac{P\left(\frac{1}{y^{\pi/\theta}}\right) - P\left(\frac{1}{(c_\pm x)^{\pi/\theta}}\right)}{(y-c_-x)(y-c_+x)}$$

and letting $y \to c_+x$ and $y \to c_-x$, one finds

$$L(h)(x,c_\pm x) = \mp\frac{\sigma_{11}}{\sigma_{22}}\frac{\pi}{\theta}\frac{1}{(c_\pm x - c_\mp x)}P'\left(\frac{1}{(c_\pm x)^{\pi/\theta}}\right)\frac{1}{(c_\pm x)^{\pi/\theta+1}}.$$

Eventually, we get

$$\begin{aligned}
&L(h)(x,c_-x) - L(h)(x,c_+x)\\
&= \frac{\sigma_{11}}{\sigma_{22}}\frac{\pi}{\theta}\left(\frac{1}{(c_+x-c_-x)}\frac{P'\left(\frac{1}{(c_+x)^{\pi/\theta}}\right)}{(c_+x)^{\pi/\theta+1}} - \frac{1}{(c_-x-c_+x)}\frac{P'\left(\frac{1}{(c_-x)^{\pi/\theta}}\right)}{(c_-x)^{\pi/\theta+1}}\right)\\
&= \frac{\sigma_{11}}{\sigma_{22}}\frac{\pi}{\theta}\left(\frac{c_+}{c_+-c_-}P'\left(\frac{1}{(c_+x)^{\pi/\theta}}\right)\frac{1}{(c_+x)^{\pi/\theta+2}} - \frac{c_-}{c_--c_+}P'\left(\frac{1}{(c_-x)^{\pi/\theta}}\right)\frac{1}{(c_-x)^{\pi/\theta+2}}\right)\\
&= -\frac{\sigma_{11}}{\sigma_{22}}\frac{\pi}{\theta}\frac{c_+c_-}{(c_+-c_-)^2}\left(P'\left(\frac{1}{(c_+x)^{\pi/\theta}}\right)\frac{1}{(c_+x)^{\pi/\theta+2}} - P'\left(\frac{1}{(c_-x)^{\pi/\theta}}\right)\frac{1}{(c_-x)^{\pi/\theta+2}}\right),
\end{aligned}$$

where the last equality follows from $(c_+x)^{\pi/\theta} = (c_-x)^{\pi/\theta}$. Therefore, the boundary value equation (22) is now homogeneous, and of the form

$$\frac{1}{2}\sigma_{11}L_1(v)(c_+x) - F(c_+x) = \frac{1}{2}\sigma_{11}L_1(v)(c_-x) - F(c_-x),$$

where F is equal on $Y_+([0,\infty]) \cup Y_-([0,\infty])$ to

$$F(y) = -\frac{\sigma_{11}}{\sigma_{22}}\frac{\pi}{\theta}\frac{c_+c_-}{(c_+-c_-)^2}P'\left(\frac{1}{y^{\pi/\theta}}\right)\frac{1}{y^{\pi/\theta+2}}. \tag{23}$$

We note that the simpler case when $F(c_+x) = F(c_-x)$ occurs exactly when $c_+^2 = c_-^2$, i.e., θ is 0 or $\pi/2$. In this way, we obtain a boundary value problem analogous to the harmonic case, which, on the boundary of $\mathcal{G}_Y$ except at 0, leads to

$$\frac{1}{2}\sigma_{11}L_1(v)(y) - F(y) = Q\left(\frac{1}{y^{\pi/\theta}}\right),$$

for any given polynomial Q. The same computation applies to $L_2(v)$. As such, using the equation (21), the Laplace transform of the bi-harmonic function v admits the following form:

▶ **Theorem 4.** *For any polynomials P and Q, the formula*

$$L(v)(x,y) = \frac{1}{\gamma(x,y)}\left[Q\left(\frac{1}{y^{\pi/\theta}}\right) - Q\left(\frac{1}{(c_+x)^{\pi/\theta}}\right) + G(x,y) + L(h)(x,y)\right]$$

is the Laplace transform $L(v)$ of a bi-harmonic function v satisfying $\mathcal{G}v = h$, where h is a harmonic function with Dirichlet boundary conditions, where the Laplace transform $L(h)$ of h has the form (20) *and where*

$$G(x,y) = F(y) - F(c_+x) - L(h)(x, c_+x),$$

with F defined in Eq. (23).

The above theorem can be understood as a Laplace transform counterpart of Almansi's theorem [1].

Recursively, if v_n is polyharmonic of order n with $\mathcal{G}v_n = v_{n-1}$, where v_{n-1} is polyharmonic of order $n-1$, the above method permits to express the Laplace transform of v_n through the one of v_{n-1}, allowing to construct polyharmonic functions via Laplace inversion.

Further computations for the Brownian motion with identity covariance matrix are proposed in Appendix A.

3 Discrete polyharmonic functions

Similarly to the continuous setting, we first investigate the appearance of polyharmonic functions in the asymptotic expansions of the counting coefficients of lattice paths with prescribed endpoints, starting from an exact expression for these coefficients (such exact expressions may typically be obtained from reflection principles). We then implement the functional equation approach to construct polyharmonic functions.

Our framework is thus the following. We consider random walks in the quarter plane $\mathbb{Z}_+^2$ with the following assumptions:

1. The walk is homogeneous with transition probabilities $\{p_{i,j}\}_{-1\leq i,j\leq 1}$ to the eight nearest neighbours and $p_{0,0} = 0$ (so we are only considering walks with small steps),
2. In the list $p_{1,1}, p_{1,0}, p_{1,-1}, p_{0,-1}, p_{-1,-1}, p_{-1,0}, p_{-1,1}, p_{0,1}$, there are no three consecutive zeros (to avoid degenerate cases),
3. The drifts $\sum_{i,j} ip_{i,j}$ and $\sum_{i,j} jp_{i,j}$ are zero.

The Markov operator P of the walk is defined on discrete functions by

$$Pf(x,y) = \sum_{-1\leq i,j\leq 1} p_{i,j} f(x+i, y+j),$$

and the Laplacian operator is $L = P - I$. A function f is said to be *harmonic* if $Lf = 0$ and *polyharmonic* of order p if $L^p f = 0$.

3.1 Examples of asymptotic expansion in walk enumeration problems

We start by recalling a few exact expressions for the number of quarter plane walks of length n with prescribed endpoints.

▶ **Example 5** (The diagonal walk). The step set is $\{\nearrow, \nwarrow, \searrow, \swarrow\}$, with uniform transition probabilities $\frac{1}{4}$. It is well known (see for instance [9]) that

$$q((i,j),(0,0);n) = \frac{(i+1)(j+1)}{\frac{n+i+2}{2}\,\frac{n+j+2}{2}}\binom{n}{\frac{n+i}{2}}\binom{n}{\frac{n+j}{2}}, \tag{24}$$

with i and j having the same parity as n. Starting from (24), one can prove that

$$q((i,j),(0,0);n) \sim \frac{8}{\pi} 4^n \sum_{p\geq 0} \frac{v_p(i,j)}{n^{3+p}}, \tag{25}$$

where the first few terms in the above asymptotic expansion are given by

$$\left\{ \begin{array}{lcl} v_0(i,j) & = & (i+1)(j+1), \\ v_1(i,j) & = & -\frac{1}{2}(i+1)(j+1)(i^2+j^2+2i+2j+9). \end{array} \right.$$

The first term v_0 is the well-known unique (up to multiplicative constants) positive harmonic function, with Dirichlet conditions; it is the same as for the simple walk, see (7) and (26). The next term satisfies $Lv_1 = -3v_0$, and therefore is bi-harmonic. Note that in fact, using the explicit expression of the Laplacian L, it is obvious that any polynomial of degree at most $2p-1$ is polyharmonic of order p, since for any polynomial f of degree k, Lf has degree at most $k-2$ (it is a discrete equivalent of Lemma 1).

To derive a full asymptotic expansion of (24), we shall use the Laplace method applied to the counting coefficients rewritten as an integral, in the spirit of [22, p. 75–79] (alternatively one can apply the saddle-point method [17, Chap. B VIII] in the framework of analytic combinatorics in several variables [14, 19]). We choose to postpone it to Appendix B, since the computations are a bit long, though straightforward.

▶ **Example 6** (The simple random walk)**.** The step set is $\{\leftarrow,\uparrow,\rightarrow,\downarrow\}$, with uniform transition probabilities $\frac{1}{4}$. We have (6) by [9]. Again, starting from (6), one can prove that

$$q((i,j),(0,0);n) \sim \frac{4}{\pi} 4^n \sum_{p\geq 0} \frac{v_p(i,j)}{n^{3+p}},$$

where the first few terms in the asymptotic expansion are

$$\left\{ \begin{array}{lcl} v_0(i,j) & = & (i+1)(j+1), \\ v_1(i,j) & = & -\frac{1}{4}(i+1)(j+1)(2i^2+2j^2+4i+4j+15). \end{array} \right. \tag{26}$$

Again, v_0 is harmonic, and since $Lv_1 = -\frac{3}{2}v_0$, v_1 is bi-harmonic.

▶ **Example 7** (The tandem walk)**.** The step set is $\{\nwarrow,\rightarrow,\downarrow\}$ with uniform transition probabilities $\frac{1}{3}$. From [10, Prop. 9], we know that:

$$q((i,j),(0,0);n) = \frac{(i+1)(j+1)(i+j+2)(3m+2i+j)!}{m!(m+i+1)!(m+i+j+2)!},$$

with $n = 3m+2i+j$. In this case, writing the asymptotic expansion

$$q((i,j),(0,0);n) \sim \frac{\sqrt{3}}{2\pi} 3^n \sum_{p\geq 0} \frac{v_p(i,j)}{n^{4+p}},$$

one has for the harmonic function v_0 and the bi-harmonic function v_1,

$$\left\{ \begin{array}{lcl} v_0(i,j) & = & (i+1)(j+1)(i+j+2), \\ v_1(i,j) & = & -\frac{1}{9}(i+1)(j+1)(i+j+2)(3i^2+3j^2+3ij+9i+9j+38). \end{array} \right. \tag{27}$$

3.2 Functional equation approach in the discrete case

We implement here the functional equation method to construct polyharmonic functions. We start by recalling the key arguments in the harmonic case; details may be found in [20].

For a harmonic function h, we denote by H its generating function, namely,

$$H(x,y) = \sum_{i,j\geq 0} h(i,j)x^i y^j.$$

The *kernel* of the random walk is defined as the polynomial

$$K(x,y) = xy\left(\sum_{-1\leq k,\ell\leq 1} p_{k,\ell}x^{-k}y^{-\ell} - 1\right).$$

The harmonic equation $Lh = 0$ yields the following *functional equation*

$$K(x,y)H(x,y) = K(x,0)H(x,0) + K(0,y)H(0,y) - K(0,0)H(0,0). \tag{28}$$

To solve (28), one first proves that the function $H(x,0)$ (and similarly $H(0,y)$) satisfies a *boundary value problem* (see [20]):

1. $H(x,0)$ is analytic in $\mathcal{G}_X$,
2. $H(x,0)$ is continuous on $\overline{\mathcal{G}_X} \setminus \{1\}$,
3. For all x in the boundary of $\mathcal{G}_X$ except at 1, $H(x,0)$ satisfies the boundary equation:

$$K(x,0)H(x,0) - K(\overline{x},0)H(\overline{x},0) = 0.$$

Here, $\mathcal{G}_X$ is a certain domain bounded by the curve $X_+([y_1,1]) \cup X_-([y_1,1])$, where $X_\pm(y)$ are the branches of the algebraic function defined by $K(X(y),y) = 0$. Indeed, writing K as

$$K(x,y) = \widetilde{\alpha}(y)x^2 + \widetilde{\beta}(y)x + \widetilde{\gamma}(y),$$

where $\widetilde{\alpha}, \widetilde{\beta}, \widetilde{\gamma}$ are polynomials of degree 2 whose coefficients depend on the model, we have

$$X_\pm(y) = \frac{-\widetilde{\beta}(y) \pm \sqrt{\widetilde{\delta}(y)}}{2\widetilde{\alpha}(y)},$$

where $\widetilde{\delta}(y) = \widetilde{\beta}(y)^2 - 4\widetilde{\alpha}(y)\widetilde{\gamma}(y)$. The functions $X_\pm$ are thus meromorphic on a cut plane, determined by the zeros of $\widetilde{\delta}$.

It follows by [20] that $K(x,0)H(x,0)$ may be written as a function of a certain conformal mapping ω (see [20, Eq. (3.1)] for its explicit expression):

$$K(x,0)H(x,0) = P(\omega(x)),$$

where P is an arbitrary entire function, for example a polynomial. This represents the analogous statement as (19) in the continuous setting. By the functional equation (28), one eventually finds that

$$H(x,y) = \frac{P(\omega(x)) - P(\omega(X_+(x)))}{K(x,y)},$$

which again should be compared with (20) in the continuous case.

For a bi-harmonic function v, satisfying $Lv = h$ with h a harmonic function, the functional equation now writes

$$K(x,y)V(x,y) = K(x,0)V(x,0) + K(0,y)V(0,y) - K(0,0)V(0,0) - xyH(x,y), \tag{29}$$

where V is the generating function of v, i.e., $V(x,y) = \sum_{i,j\geq 0} v(i,j)x^i y^j$; compare with (21). Notice that the equation (29) is very close to functional equations coming up in walk enumeration problems.

Plugging the roots of the kernel into (29), one has

$$K(X_\pm(y),0)V(X_\pm(y),0) + K(0,y)V(0,y) - K(0,0)V(0,0) - X_\pm(y)yH(X_\pm(y),y) = 0,$$

which leads to the boundary equation

$$K(x,0)V(x,0) - K(\overline{x},0)V(\overline{x},0) = y\left(xH(x,y) - \overline{x}H(\overline{x},y)\right), \tag{30}$$

for x on the boundary of $\mathcal{G}_X$ (except at 1).

Note that a general method to solve this kind of boundary value problem (30) exists [16], for any quantity in the right-hand side, ending up in some contour integral expression for the unknown function $K(x,0)V(x,0)$. We choose to provide below examples with simpler, integral-free expressions. Indeed, the resolution of (30) is made easier in some peculiar cases, for instance when the right-hand side of (30) is zero (which occurs for the simple random walk, see Example 6 below), or when it can be decoupled in the terminology of [6] (which is analogous to the continuous setting and holds for the tandem walk, see Appendix C).

▶ **Example 6** (continued). We consider here the case of the simple random walk,with kernel

$$K(x,y) = xy\left(\frac{1}{4}\left(x + \frac{1}{x} + y + \frac{1}{y}\right) - 1\right).$$

The domain $\mathcal{G}_X$ is the open unit disk, and the conformal mapping ω admits the expression $\omega(x) = \frac{x}{(1-x)^2}$, see [20]. A computation shows that $\omega(X_+(y)) = -\omega(y)$, thus one gets that the generating function of a harmonic function h may be written as

$$H(x,y) = \frac{P(\omega(x)) - P(-\omega(y))}{K(x,y)}.$$

Choosing $P(x) = \frac{x}{4}$ leads to

$$H(x,y) = \frac{\frac{\frac{1}{4}x}{(1-x)^2} + \frac{\frac{1}{4}y}{(1-y)^2}}{xy\left(\frac{1}{4}(x + \frac{1}{x} + y + \frac{1}{y}) - 1\right)} = \frac{1}{(1-x)^2(1-y)^2} = \sum_{i,j\geq 0}(i+1)(j+1)x^i y^j,$$

that is, H is the generating function of the unique positive harmonic function, see (26).

We now consider bi-harmonic functions. Using the explicit form of H, one sees that the right-hand side of Eq. (30) vanishes. Indeed, we have

$$\begin{aligned}X_+(y)&H(X_+(y),y) - X_-(y)H(X_-(y),y)\\ &= X_+(y)\frac{P'(\omega(X_+(y)))\omega'(X_+(y))}{\widetilde{\alpha}(y)(X_+(y)-X_-(y))} - X_-(y)\frac{P'(\omega(X_-(y)))\omega'(X_-(y))}{\widetilde{\alpha}(y)(X_-(y)-X_+(y))},\end{aligned}$$

which is equal to zero since $\omega(X_+(y)) = \omega(X_-(y))$ and

$$X_+(y)\frac{\omega'(X_+(y))}{X_+(y)-X_-(y)} - X_-(y)\frac{\omega'(X_-(y))}{X_-(y)-X_+(y)} = 0$$

by straightforward computations. The boundary equation has thus exactly the same form as the one in the harmonic case, so we get that on the boundary of $\mathcal{G}_X$,

$$K(x,0)V(x,0) = Q(\omega(x)),$$

for some polynomial Q. Using (twice) the functional equation (29), the general form for the generating function of a bi-harmonic v satisfying $Lv = h$, with h harmonic, is thus

$$V(x,y) = \frac{Q(\omega(x)) - Q(-\omega(y)) + X_+(y)yH(X_+(y),y) - xyH(x,y)}{K(x,y)},$$

with

$$H(x,y) = \frac{P(\omega(x)) - P(-\omega(y))}{K(x,y)} \quad \text{and} \quad H(X_+(y),y) = \frac{P'(\omega(X_+(y)))\omega'(X_+(y))}{\widetilde{\alpha}(y)(X_+(y) - X_-(y))}.$$

For instance, taking $P(x) = x$ and Q the zero polynomial leads to the bi-harmonic function (non symmetrical in i and j)

$$v(i,j) = (i+1)j(j+1)(j+2).$$

Indeed, one has

$$X_+(y)H(X_+(y),y) = -\frac{y}{(1-y)^4},$$

so the generating function V writes

$$V(x,y) = \frac{-4y}{(1-x)^2(1-y)^4},$$

which is easily inverted. On the other hand, taking $P(x) = x$ and $Q(x) = -2x^2 - \frac{5}{2}x$, one obtains the bi-harmonic function

$$v(i,j) = (i+1)(j+1)(2i^2 + 2j^2 + 4i + 4j + 15),$$

which is (up to a multiplicative constant) the bi-harmonic function v_1 appearing in Eq. (26). Another example will be treated in Appendix C.

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A Detailed computations for the standard Brownian motion in the quadrant

Here we apply the functional equation approach to the case of the Brownian motion in the quarter plane with identity covariance matrix. The kernel γ is equal to $\gamma(x,y) = \frac{1}{2}\left(x^2+y^2\right)$, so $c_\pm = \pm i$ and $\theta = \frac{\pi}{2}$, see (18). The functional equation (17) for h harmonic is then

$$(x^2+y^2)L(h)(x,y) = L_1(h)(y) + L_2(h)(x),$$

which leads to

$$L(h)(x,y) = \frac{P\left(\frac{1}{y^2}\right) - P\left(-\frac{1}{x^2}\right)}{x^2+y^2}.$$

In case when P is the degree 1 polynomial $P(x) = x$, one gets $L(h)(x,y) = \frac{1}{x^2y^2}$ which is the Laplace transform of the well-known unique positive harmonic function within the quarter plane $h(x,y) = xy$.

More generally, the choice of $P(x) = -(2j)!(-x)^j$ leads to the Laplace transform (in Cartesian coordinates) of the harmonic function $f_{2j,j}$ defined in (14). Indeed, recall that $f_{2j,j}(\rho,\theta) = \rho^{2j}\sin(2j\theta)$, which is written in Cartesian coordinates as follows. Recall that the Chebyshev polynomial U_j of the second kind is defined as $U_j(\cos\theta)\sin\theta = \sin(j\theta)$, $j \geq 0$, and admits the expression

$$U_j(z) = z^j \sum_{k=0}^{\lfloor j/2 \rfloor} \binom{j+1}{2k+1}(1-z^{-2})^k.$$

Hence, thanks to the explicit expression of U_{2j-1}, the harmonic function $f_{2j,j}$ can be written, in Cartesian coordinates $(x,y) = (\rho\cos\theta, \rho\sin\theta)$,

$$f_{2j,j}(x,y) = \sum_{k=0}^{j-1}(-1)^k \binom{2j}{2k+1} y^{2k+1}x^{2j-(2k+1)}.$$

The Laplace transform of $f_{2j,j}$ is now computed using $L(x^n y^k) = \frac{n!k!}{x^{n+1}y^{k+1}}$, and one obtains

$$L(f_{2j,j})(x,y) = (2j)!\sum_{k=0}^{j-1}(-1)^k \frac{1}{y^{2k+2}x^{2j-2k}} = (2j)!\frac{\left(\frac{1}{x^2}\right)^j - \left(-\frac{1}{y^2}\right)^j}{x^2+y^2}. \tag{31}$$

For v bi-harmonic, the functional equation (21) is

$$(x^2+y^2)L(v)(x,y) = L_1(v)(y) + L_2(v)(x) + 2L(h)(x,y),$$

and the general form of the Laplace transform of v writes

$$L(v)(x,y) = \frac{Q\left(\frac{1}{y^2}\right) - Q\left(-\frac{1}{x^2}\right) + \frac{2}{x^4}P'\left(-\frac{1}{x^2}\right) + 2\frac{P\left(\frac{1}{y^2}\right)-P\left(-\frac{1}{x^2}\right)}{x^2+y^2}}{x^2+y^2}, \tag{32}$$

where P and Q are arbitrary polynomials. Choosing $P(x)$ equal to x and $Q(x)$ of degree 2, equal to x^2, gives that

$$L(v)(x,y) = \frac{x^2+y^2}{x^4y^4} = \frac{1}{x^2y^4} + \frac{1}{x^4y^2},$$

which is the Laplace transform of the function $v(x,y) = (x^2+y^2)xy$, which corresponds in polar coordinate (ρ,θ) to the bi-harmonic function $f_{4,2}(\rho,\theta) = \rho^4\sin 2\theta$ defined in (14).

More generally, choosing

$$P(x) = (-1)^{j+1}(2j)!2(2j+1)x^j \quad \text{and} \quad Q(x) = (-1)^{j+1}(2j)!2(2j+1)jx^{j+1}$$

leads to the bi-harmonic function $f_{2j+2,j}$. Indeed, since $f_{2j+2,j}(x,y) = (x^2+y^2)f_{2j,j}(x,y)$, one has, from the usual properties of the Laplace transform, that $L(f_{2j+2,j}) = \Delta L(f_{2j,j})$. As such, by applying the Laplacian to the Laplace transform of $f_{2j,j}$ given in (31), one obtains that

$$L(f_{2j+2,j})(x,y) = \frac{(2j)!2(2j+1)}{x^2y^2(x^2+y^2)^2}\left\{(j+2)x^2y^2\left(\left(\frac{1}{x^2}\right)^j - \left(\frac{-1}{y^2}\right)^j\right) + j\left(y^4\left(\frac{1}{x^2}\right)^j - x^4\left(\frac{-1}{y^2}\right)^j\right)\right\}.$$

Now, plugging the above choice of P and Q in Eq. (32) gives easily the formula.

B Complete asymptotic expansion for the diagonal walk

As an explicit example, we provide a complete asymptotic expansion for the number (24) of n-excursions from the origin to (i,j) for the diagonal walk with steps from $\{\nearrow,\nwarrow,\searrow,\swarrow\}$. A straightforward way to obtain such an asymptotic expansion is to apply the standard Laplace's method (see [17, p. 755]) using an integral representation of (24) (in [22, p. 75–79], this is applied to obtain first order asymptotic estimates in lattice paths enumeration problems). This leads to an explicit new family of polynomials $(v_p)_{p\geq 0}$ of increasing degree, where v_p is the polyharmonic function of order $p+1$ appearing in the expansion (25), see Corollary 9.

Let us first introduce the necessary notations. Projecting the walk onto the coordinate axes, one gets two decoupled prefixes of Dyck paths. Hence (24) is obtained by a simple application of the reflection principle in the one-dimensional case, which gives that the number of non-negative paths from 0 to λ with n steps is given by

$$m(\lambda,n) := \binom{n}{\frac{n+\lambda}{2}} - \binom{n}{\frac{n+\lambda+2}{2}} = \frac{\lambda+1}{\frac{n+\lambda+2}{2}}\binom{n}{\frac{n+\lambda}{2}}, \tag{33}$$

with $\lambda \equiv n \mod 2$. Using the simple integral representation of the binomial coefficient

$$\binom{n}{k} = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ikt}(1+e^{it})^n dt,$$

one readily obtains the following integral representation for $m(\lambda,n)$:

$$m(\lambda,n) = \frac{2}{\pi}\int_{-\pi/2}^{\pi/2} 2^n(\cos y)^n \sin((\lambda+1)y)\sin(y)dy. \tag{34}$$

Now define the sequence $(\alpha(m))_{m\geq 1}$ as

$$\alpha(m) = \frac{(4^m-1)|B_{2m}|2^{2m}}{2m(2m)!}, \tag{35}$$

where the B_{2m}'s are the Bernoulli numbers, which can be defined through the Riemann zeta function at even integers:

$$\zeta(2m) = \frac{|B_{2m}|(2\pi)^{2m}}{2(2m)!}.$$

Define also, for $s \geq k \geq 0$,

$$B^{\alpha}_{s,k} := B_{s,k}\left(\alpha(2),\ldots,\alpha(s-k+2)\right), \tag{36}$$

the rational numbers obtained by evaluating the partial ordinary Bell polynomial in the variables $\alpha(m+1)$. Recall that by definition, see for instance [13], the partial ordinary Bell polynomials in the variables $(x_k)_{k\geq 1}$ are the polynomials obtained by performing the formal double series expansion:

$$\exp\left(u\sum_{m\geq 1} x_m t^m\right) = \sum_{n\geq k\geq 0} B_{n,k}(x_1,\ldots,x_{n-k+1})t^n\frac{u^k}{k!}.$$

Note that the polynomial $B_{n,k}$ contains $p(n,k)$ monomials, where $p(n,k)$ stands for the number of partitions of n into k parts, see [13] for details and for an explicit expression of these polynomials. Finally, define for $p \geq k \geq 0$,

$$C^{\alpha}_{k,p} = \frac{1}{k!}\sum_{j=k}^{p}\frac{(-1)^j}{(2p-2j+1)!}B^{\alpha}_{j,k}. \tag{37}$$

We first give a complete asymptotic expansion for prefixes of Dyck paths.

▶ **Theorem 8.** *Let $m(\lambda, n)$ be the number of non-negative paths from 0 to $\lambda \in \mathbb{Z}_+$ given by (33). The following asymptotic expansion holds as $n \to \infty$:*

$$m(\lambda, n) \sim 2\sqrt{2}\frac{2^n}{\sqrt{\pi}}\frac{1}{n^{3/2}}\sum_{j\geq 0}\frac{(-1)^j}{n^j}h_j(\lambda),$$

where for $j \geq 0$,

$$h_j(\lambda) = \sum_{p=0}^{j}\sum_{k=0}^{p}\frac{(-1)^k}{(2(j-p)+1)!}C^{\alpha}_{k,p}m_{2(k+j+1)}(\lambda+1)^{2(j-p)+1}, \tag{38}$$

where $m_{2k} = \frac{(2k)!}{2^k k!}$ is the $2k$-th Gaussian moment and $C^{\alpha}_{k,p}$ is defined in (37).

Hence, the above theorem gives, in the one-dimensional case, an asymptotic expansion of the number of non-negative paths in terms of polyharmonic functions. Indeed, it is easily seen that the polynomial h_j has degree $2j+1$, so is polyharmonic of order $j+1$ for the one-dimensional Laplacian $Lf(x) = \frac{1}{2}(f(x+1)+f(x-1)) - f(x)$.

Since the number of n-excursions for the diagonal walk is the product of two numbers of (decoupled) Dyck paths, one readily obtains the following corollary.

▶ **Corollary 9.** *Let $q(0,(i,j);n)$ be the number of diagonal paths with n steps from the origin to (i,j) and confined in the quadrant, given by (24). Then*

$$q(0,(i,j);n) \sim \frac{8}{\pi}\frac{1}{n^3}4^n\sum_{p\geq 0}\frac{(-1)^p}{n^p}v_p(i,j),$$

where, with h_k defined in (38),

$$v_p(i,j) = \sum_{k=0}^{p}h_k(i)h_{p-k}(j).$$

Clearly, the polynomial function v_p has degree $2p+1$ and thus is polyharmonic of order $p+1$ for the Laplacian associated to the diagonal walk. The set of exponents (16) appearing in the asymptotic expansion is here $3+\mathbb{N}$.

Proof of Theorem 8. To obtain the claimed asymptotic expansion, we apply the Laplace method as in [17, p. 755] to the integral representation of $m(\lambda, n)$ in (34). Indeed, the cosine function admits only one maximum in the interval $[-\frac{\pi}{2}, \frac{\pi}{2}]$, at $y = 0$, and the contribution to the integral outside any fixed segment containing 0 is exponentially small and as such can be discarded for an asymptotic consideration.

So, first, we perform the change of variable $\theta = \frac{y}{\sqrt{n}}$ to get

$$m(\lambda, n) = 2^n\frac{2}{\pi}\frac{1}{n^{1/2}}\int_{-\frac{\pi}{2}\sqrt{n}}^{\frac{\pi}{2}\sqrt{n}}\cos\left(\frac{y}{\sqrt{n}}\right)^n\sin\left(\frac{y}{\sqrt{n}}\right)\sin\left((\lambda+1)\frac{y}{\sqrt{n}}\right)dy.$$

The next step is to consider an asymptotic expansion of the integrand as $n \to \infty$. Using the Weierstrass product formula for the cosine function,

$$\cos y = \prod_{k=1}^{\infty}\left(1 - \frac{4y^2}{\pi^2(2k-1)^2}\right)$$

and the Taylor series of the logarithm function, one has

$$\log\cos(y) = -\sum_{m\geq 1}\alpha(m)y^{2m},$$

where the sequence $(\alpha(m))_{m\geq 1}$ is defined in (35). Note that an interpretation of the sequence $(\alpha(m))_{m\geq 1}$ is that they correspond to the cumulant sequence of the Bernoulli distribution $\frac{1}{2}\delta_{+1}+\frac{1}{2}\delta_{-1}$. Now one has, using $\alpha(1)=\frac{1}{2}$ and the Taylor series of the exponential function,

$$\cos\left(\frac{y}{\sqrt{n}}\right)^n = \exp\left(n\log\cos\left(\frac{y}{\sqrt{n}}\right)\right) = e^{-y^2/2}\sum_{s\geq 0}\frac{1}{n^s}\sum_{k=0}^{s}\frac{(-1)^k}{k!}B^{\alpha}_{s,k}\, y^{2(k+s)},$$

where $B^{\alpha}_{s,k}$ is the partial ordinary Bell polynomial defined in (36). Now, using the Taylor series of the sine function, and after some elementary manipulations, one gets

$$\begin{aligned}\cos&\left(\frac{y}{\sqrt{n}}\right)^n \sin\left(\frac{y}{\sqrt{n}}\right)\sin\left((\lambda+1)\frac{y}{\sqrt{n}}\right)\\ &= e^{-y^2/2}\frac{1}{n}\sum_{j\geq 0}\frac{(-1)^j}{n^j}\sum_{p=0}^{j}\sum_{k=0}^{p}(-1)^k\frac{C^{\alpha}_{k,p}}{(2(j-p)+1)!}y^{2(k+j)+2}(\lambda+1)^{2(j-p)+1},\end{aligned}$$

where $C^{\alpha}_{k,p}$ is defined in (37).

The next step in the Laplace method is to neglect the tails. Hence, we write

$$m(\lambda,n)\sim\frac{2}{\pi}\frac{2^n}{n^{3/2}}\sum_{j\geq 0}\frac{(-1)^j}{n^j}\sum_{p=0}^{j}\sum_{k=0}^{p}\frac{(-1)^k C^{\alpha}_{k,p}}{(2(j-p)+1)!}(\lambda+1)^{2(j-p)+1}\int_{-\kappa_n}^{\kappa_n}e^{-y^2/2}y^{2(k+j)+2}dy,$$

where κ_n is chosen so that the error bounds are exponentially small (for instance one can choose arbitrarily $\kappa_n = n^{1/10}$). Completing the tails of the Gaussian integral, that is

$$\begin{aligned}\int_{-\kappa_n}^{\kappa_n}e^{-y^2/2}y^{2(k+j)+2}dy \sim \int_{\mathbb{R}}e^{-y^2/2}y^{2(k+j)+2}dy &= \sqrt{2\pi}\frac{(2(k+j+1))!}{2^{k+j+1}(k+j+1)!}\\ &= \sqrt{2\pi}m_{2(k+j+1)},\end{aligned}$$

where $m_{2k}=\frac{(2k)!}{2^k k!}$ is the $2k$-th Gaussian moment, one finally obtains, with h_j defined in (38), that

$$m(\lambda,n)\sim 2\sqrt{2}\frac{2^n}{\sqrt{\pi}}\frac{1}{n^{3/2}}\sum_{j\geq 0}\frac{(-1)^j}{n^j}h_j(\lambda).$$ ◀

C The example of tandem walks

In this subsequent example, we consider the tandem walk with steps from $\{\nwarrow,\rightarrow,\downarrow\}$, see Example 7. In this case, the functional equation approach admits a nicer form because the right-hand side of Eq. (30) can be decoupled, that is, can be written as $G(X_+(y))-G(X_-(y))$, for some function G. The computations are close to the continuous case but are quite tedious. First, we know [20] that the generating function H of a harmonic function h is of the form

$$H(x,y)=\frac{P(\omega(x))-P(\omega(X_+(y)))}{K(x,y)}, \tag{39}$$

where the conformal mapping ω is given by $\omega(x)=\frac{x^2}{(1-x)^3}$. The unique positive harmonic function $v_0(i,j)=\frac{1}{2}(i+1)(j+1)(i+j+2)$ of (27) is obtained choosing $P(x)=\frac{1}{3}x$.

Using the general form of H, one has

$$yX_+(y)H(X_+(y),y) - yX_-(y)H(X_-(y),y) = \\ 3\frac{yX_+(y)\omega'(X_+(y))}{X_+(y)-X_-(y)}P'(\omega(X_+(y))) - 3\frac{yX_-(y)\omega'(X_-(y))}{X_-(y)-X_+(y)}P'(\omega(X_-(y))).$$

Define now the *decoupling* function on $\mathcal{G}_X$:

$$F(x) = -\frac{x^3}{(1-x)^6}. \tag{40}$$

Some computations show that

$$\frac{yX_+(y)\omega'(X_+(y))}{X_+(y)-X_-(y)} - \frac{yX_-(y)\omega'(X_-(y))}{X_-(y)-X_+(y)} = F(X_+(y)) - F(X_-(y)).$$

A crucial point is to *guess* the function F in (40) satisfying the above equation. Minding the fundamental fact that $\omega(X_+(y)) = \omega(X_-(y))$, it follows that

$$yX_+(y)H(X_+(y),y) - yX_-(y)H(X_-(y),y) = G(X_+(y)) - G(X_-(y)),$$

where $G(x) = 3F(x)P'(\omega(x))$. One deduces that the generating function $V(x,y)$ for a bi-harmonic function v satisfying $Lv = h$ admits the form

$$\frac{1}{K(x,y)}\Big(Q(\omega(x)) - Q(\omega(X_+(y))) + G(x) - G(X_+(y)) + X_+(y)yH(X_+(y),y) - xyH(x,y)\Big),$$

where H has the general form given by Eq. (39) and $G(x) = 3F(x)P'(\omega(x))$ with the decoupling function F defined in Eq. (40). Note that this has to be compared with Theorem 4.

Choosing $P(x) = x$ and $Q = 0$ leads to the bi-harmonic function

$$v(i,j) = (j+1)(i+1)(i+j+2)(2i^3+3i^2j+14i^2+5ij+24i-3ij^2-2j^3-4j^2+6j). \tag{41}$$

To obtain to bi-harmonic function v_1 of (27), one chooses $P(x) = -\frac{8}{9}x$ and $Q(x) = \frac{8}{3}x^2 + \frac{76}{27}x$. This is obtained by noticing that an appropriate linear combination of the bi-harmonic function (41) and of v_1 is harmonic and its generating function corresponds to the term

$$\frac{Q(\omega(x)) - Q(\omega(X_+(y)))}{K(x,y)}.$$

As such, computing its generating function leads to the polynomial Q.

Cut Vertices in Random Planar Maps

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Abstract

The main goal of this paper is to determine the asymptotic behavior of the number X_n of cut-vertices in random planar maps with n edges. It is shown that $X_n/n \to c$ in probability (for some explicit $c > 0$). For so-called subcritial subclasses of planar maps like outerplanar maps we obtain a central limit theorem, too.

2012 ACM Subject Classification Mathematics of computing → Random graphs

Keywords and phrases random planar maps, cut vertices, generating functions, local graph limits

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.10

Funding *Michael Drmota*: Research supported by the Austrian Science Foundation FWF, project F50-02.
Marc Noy: Research supported in part by Ministerio de Ciencia, Innovación y Universidades MTM2017-82166-P.

Acknowledgements We thank the referees for their careful reading and their valuable comments for improving the presentation.

1 Introduction

A *planar map* is a connected planar graph, possibly with loops and multiple edges, together with an embedding in the plane. A map is *rooted* if a vertex v and an edge e incident with v are distinguished, and are called the *root-vertex* and *root-edge*, respectively. Sometimes the root-edge is considered as directed away from the root-vertex. In this sense, the face to the right of e is called the *root-face* and is usually taken as the outer face. All maps in this paper are rooted.

The enumeration of rooted maps is a classical subject, initiated by Tutte in the 1960's. Tutte (and Brown) introduced the technique now called "the quadratic method" in order to compute the number M_n, $n \in \mathbb{N}$, of rooted maps with n edges, proving the formula

$$M_n = \frac{2(2n)!}{(n+2)!n!}3^n.$$

This was later extended by Tutte and his school to several classes of planar maps: 2-connected, 3-connected, bipartite, Eulerian, triangulations, quadrangulations, etc.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 10; pp. 10:1–10:18
Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

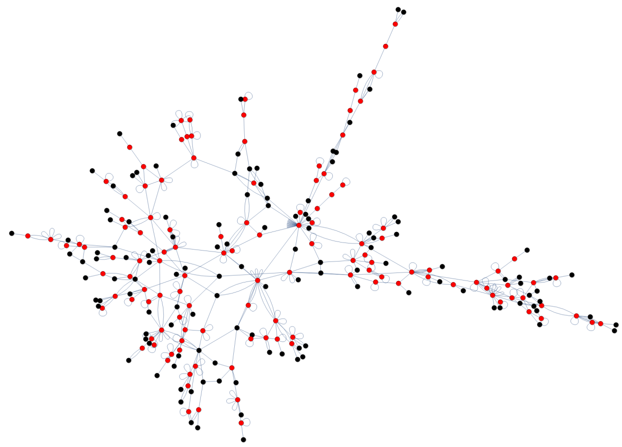

Figure 1 A randomly generated planar map with 500 edges, embedded using a spring-electrical method. Cut vertices are coloured red.

The standard random model is to assume that every map with n edges appears with the same probabiltiy $1/M_n$. Within this random setting several shape parameters of random planar maps have been studied so far, see for example [2, 8, 10, 9]. However, the number of cut vertices does not appear to have been studied. (A cut vertex is a vertex that disconnects a graph when it is removed). Figure 1 displays a randomly generated planar map with cut vertices coloured red. It is natural to expect that the number of cut vertices is asymptotically linear – and this is in fact true.

▶ **Theorem 1.** *Let X_n denote the number of cut vertices in random planar maps with n edges. Then we have*

$$\frac{X_n}{n} \xrightarrow{p} \frac{5-\sqrt{17}}{4} \approx 0.219223594.$$

Moreover, we have $\mathbb{E}[X_n] = (5-\sqrt{17})/4 \cdot n + O(1)$.

We provide two different approaches for Theorem 1. First, by a probabilistic approach, that makes use of the local convergence of random planar maps re-rooted at a uniformly selected vertex (see Section 3). Second, by a combinatorial approach based on generating functions and singularity analysis (see Section 4). The combinatorial approach yields additional information on related generating functions and on error terms, and one obtains more precise information on the expected value (see Section 4).

We conjecture that the number X_n additionally satisfies a normal central limit theorem. The intuition behind this is that X_n may be written as the sum of n seemingly weakly dependent indicator variables. The conjecture is backed up by numerical simulations we carried out, see the histogram in Figure 2. Sampling over $2 \cdot 10^5$ planar maps with $n = 5 \cdot 10^5$ edges, we obtained an average value of approximately $\mathbf{0.219223}677 \cdot n$ cut vertices. This value is already very close to the exact asymptotic value obtained in Theorem 1. The variance was approximately $0.082788 \cdot n$. It is actually possible to extend our combinatorial approach and the corresponding asymptotic analysis to second moments that leads to the precise asympotic behavior of the variance (details will be given in the journal version of this Extended Abstract).

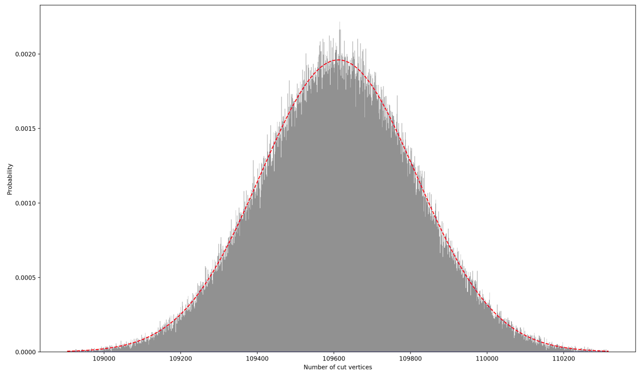

Figure 2 Histogram for the number of cut vertices in more than $2 \cdot 10^5$ randomly generated planar maps with $n = 5 \cdot 10^5$ edges each.

One important property of random planar maps that we will use in the proof of Theorem 1 is that it has a *giant 2-connected component* of linear size. There are, however, several interesting subclasses of planar maps, for example outerplanar maps (that is, all vertices are on the outer face), where all 2-connected components are (in expectation) of bounded size. Informally this means that on a global scale the map looks more or less like a tree. Such classes of maps are called subcritical – we will give a precise definition in Section 2.

▶ **Theorem 2.** *Let X_n denote the number of cut vertices in random outerplanar (or bipartite outerplanar) maps of size n. Then X_n satisfies a central limit theorem of the form*

$$\frac{X_n - cn}{\sqrt{\sigma^2 n}} \xrightarrow{d} N(0,1)$$

where $c = 1/4$ and $\sigma^2 = 5/32$ in the outerplanar case and $c = (\sqrt{3}-1)/2$ and $\sigma^2 = (11\sqrt{3}-17)/12$ in the bipartite outerplanar case.

We will give a generating function based proof for the case of outerplanar graphs in Section 5. (The proof for the bipartite outerplanar case is very similar to that.)

2 Generating Functions for Planar Maps

The generating function of planar maps is given by

$$M(z) = \sum_{n \ge 0} M_n z^n = \frac{18z - 1 + (1-12z)^{3/2}}{54z^2} = 1 + 2z + 9z^2 + 54z^3 + \cdots, \tag{1}$$

This can be shown in various ways, for example by the so-called quadratic method, where it is necessary to use an additional *catalytic variable* u that takes care of the root face valency. The corresponding generating function $M(z,u)$ (u takes care of the root face valency or equivalently by duality of the root degree) satisfies then

$$M(z,u) = 1 + zu^2 M(z,u)^2 + uz \frac{uM(z,u) - M(z)}{u-1} \tag{2}$$

which follows from a combinatorial consideration (removal of the root edge). Then this relation can be used to obtain (1) and to solve the counting problem. We refer to [11, Sec. VII. 8.2.].

Similarly it is possible to count also the number of non-root faces (with an additional variable x) which leads to the relation[1]

$$M(z,x,u) = 1 + zu^2 M(z,x,u)^2 + uzx\frac{uM(z,x,u) - M(z,x,1)}{u-1}.$$

Note that by duality $M(z,x,1)$ can be also seen as the generating function that is related to edges and non-root vertices of planar maps.

A planar map is 2-connected if it does not contain cut vertices. There are various ways to obtain relations for the corresponding generating function $B(z,x,u)$ of 2-connected planar maps – as above z takes care of the number of edges, x of the number of non-root faces, and u of the valency of the root face. By using the fact, that a 2-connected planar map, where we delete the root edge, decomposes into a sequence of 2-connected maps or single edges, we obtain the relation

$$B(z,x,u) = zxu\frac{\frac{uB(z,x,1)-B(z,x,u)}{1-u} + zu}{1 - \frac{uB(z,x,1)-B(z,x,u)}{1-u} - zu}. \tag{3}$$

We can use, for example, the quadratic method to solve this equation or we just check that we have

$$\begin{aligned} B(z,x,u) = &-\frac{1}{2}\left(1 - (1+U-V+UV-2U^2V)u + U(1-V)^2u^2\right) \\ &+ \frac{1}{2}(1-(1-V)u)\sqrt{1-2U(1+V-2UV)u + U^2(1-V)^2u^2}, \end{aligned} \tag{4}$$

where $U = U(x,y)$ and $V = V(x,y)$ are given by the algebraic equations

$$z = U(1-V)^2, \qquad xz = V(1-U)^2. \tag{5}$$

Note that in the above counting procedure we do not take the one-edge map (nor the one-edge loop) into account. Therefore we have to add the term zu on the right hand side in order to cover the case of a single edges that might occur in the above mentioned decomposition into a sequence of 2-connected maps or single edges.

Sometimes it is more convenient to include the one-edge map as well as the one-edge loop to 2-connected maps (since they have no cut-points) which leads us to the alternative generating function

$$A(z,x,u) = B(z,x,u) + zxu + zu^2.$$

Now a general rooted planar map can be obtained from a 2-connected rooted map (including the one-edge map as well as the one-edge loop) by adding to every corner a rooted planar map (a *corner* of a planar map is the angle region between two adjacent half-edges of the same vertex – note that there are $2n$ corners if there are n edges):

$$M(z,x,u) = 1 + A\left(zM(z,x,1)^2, x, \frac{uM(z,x,u)}{M(z,x,1)}\right). \tag{6}$$

[1] By abuse of notation we will use for simplicity for $M(z)$, $M(z,u)$, $M(z,x,u)$ the same symbol.

If $x = 1$ then $V(z,1)$ (and $U(z,1)$) satisfies the equation $z = V(1-V)^2$ and, thus, the dominant singularity of $V(z,1)$ (and $U(z,1)$) is $z_0 = \frac{4}{27}$, and we also have $V(z_0,1) = \frac{1}{3}$ (as well as $U(z_0,1) = \frac{1}{3}$). Hence, from (4) it follows that the function $A(z,1,1)$ has its dominant singularity at $z_0 = \frac{4}{27}$, too. On the other hand, by (1) $M(z)$ has its dominant singularity at $z_1 = \frac{1}{12}$ and we also have $M(z_1) = \frac{4}{3}$. Since $z_1 M(z_1)^2 = \frac{4}{27} = z_0$, the singularities of $M(z)$ and $A(z,1,1)$ interact. We call such a situation *critical*.

The relation (6) can also be seen as a way how all planar maps can be constructed (recursively) from 2-connected planar maps – which reflects the block-decomposition of a connected graph into its 2-connected components. Actually this principle holds, too, for several sub-classes of planar maps. As an example we consider outerplanar maps – these are maps, in which all vertices are on the outer face. Here the generating function $M_O(z)$ of outerplanar (rooted) maps satisfies

$$M_O(z) = \frac{z}{1 - A_O(M(z))}, \tag{7}$$

where $A_O(z)$ is the generating function for polygon dissections (plus a single edge) where z marks non-root vertices, which satisfies

$$2A_O(z)^2 - (1+z)A_O(z) + z = 0. \tag{8}$$

Note that the dominant singularity of $A_O(z)$ is $z_{0,O} = 3 - 2\sqrt{2}$, whereas the dominant singularity of $M_O(z)$ is $z_{1,O} = \frac{1}{8}$ and we have $M_O(z_{1,O}) = \frac{1}{18}$. So we clearly have

$$M_O(z_{1,O}) < z_{0,O}, \tag{9}$$

so that the singularities of $M_O(z)$ and $A_O(z)$ do not interact. Such a situation is called *subcritical*.

3 A probabilistic approach to cut vertices of random planar maps

We let M_n denote the uniform random planar map with n edges. It is known that M_n and related models of random planar maps admit local limits that describe the asymptotic vicinity of a typical corner, see [16, 1, 13, 4, 6, 15].

In a recent work by Drmota and Stufler [9, Thm. 2.1], a related limit object M_∞ was constructed that describes the asymptotic vicinity of a uniformly selected *vertex* v_n of M_n instead. That is, M_∞ is a random infinite but locally finite planar map with a marked vertex such that

$$(\mathsf{M}_n, v_n) \xrightarrow{d} \mathsf{M}_\infty \tag{10}$$

in the local topology.

In the present section we provide a probabilistic proof of Theorem 1. There are two steps. The first proves a law of large numbers for the number X_n of cut vertices in M_n without determining the limiting constant explicitly:

▶ **Lemma 3.** *We have $X_n/n \xrightarrow{p} p/2$, with $p > 0$ the probability that the root of M_∞ is a cut vertex.*

The factor $1/2$ originates from the fact that the number of vertices in the random map M_n has order $n/2$. We prove Lemma 3 in Section 3.4 below. In the second step, we determine this limiting probability (the proof is given in Section 3.6),

▶ **Lemma 4.** *It holds that $p = \frac{5-\sqrt{17}}{2}$.*

3.1 The local topology

We briefly recall the background related to local limits. Consider the collection $\mathfrak{M}$ of vertex-rooted locally finite planar maps. For all integers $k \geq 0$ we may consider the projection $U_k : \mathfrak{M} \to \mathfrak{M}$ that sends a map from $\mathfrak{M}$ to the submap obtained by restricting to all vertices with graph distance at most k from the root vertex. The local topology is induced by the metric

$$d_{\mathfrak{M}}(M_1, M_2) = \frac{1}{1 + \sup\{k \geq 0 \mid U_k(M_1) = U_k(M_2)\}}, \qquad M_1, M_2 \in \mathfrak{M}.$$

It is well-known that the metric space $(\mathfrak{M}, d_{\mathfrak{M}})$ is a Polish space. A limit of a sequence of vertex rooted maps in $\mathfrak{M}$ is called a local limit. The vertex rooted map (M_n, v_n) is a random point of the space of $\mathfrak{M}$, and hence the standard probabilistic notions for different types of convergence (such as distributional convergence in (10)) of random points in Polish spaces apply.

3.2 Continuity on a subset

We consider the indicator variable $f : \mathfrak{M} \to \{0, 1\}$ for the property, that the root vertex is a cut vertex.

Note that f is not continuous on $\mathfrak{M}$. Therefore we consider the subset $\Omega \subset \mathfrak{M}$ of all locally finite vertex-rooted maps with the property, that either the root is not a cut vertex, or it is a cut vertex and deleting it creates at least one finite connected component.

▶ **Lemma 5.** *The indicator variable f is continuous on Ω.*

Proof. Let $(M_n)_{n\geq 1}$ denote a sequence in $\mathfrak{M}$ with a local limit $M = \lim_{n\to\infty} M_n$ that satisfies $M \in \Omega$. If the root of M is not a cut vertex, then there is a finite cycle containing it, and this cycle must then be already present in M_n for all sufficiently large n. Hence in this case $\lim_{n\to\infty} f(M_n) = 0 = f(M)$. If the root of M is a cut vertex, then $M \in \Omega$ implies that removing it creates a finite connected component, and this component must then also be separated from the remaining graph when removing the root vertex of M_n for all sufficiently large n. Thus, $\lim_{n\to\infty} f(M_n) = 1 = f(M)$. This shows that f is continuous on Ω. ◀

Note that by similar arguments it follows that the subset Ω is closed.

3.3 Random probability measures

The collection $\mathbb{M}_1(\mathfrak{M})$ of probability measures on the Borel sigma algebra of $\mathfrak{M}$ is a Polish space with respect to the weak convergence topology.

For any finite planar map M with k vertices we may consider the uniform distribution on the k different rooted versions of M. If the map M is random, then this is a random probability measure, and hence a random point in the space $\mathbb{M}_1(\mathfrak{M})$. In particular, the conditional law $\mathbb{P}((\mathsf{M}_n, v_n) \mid \mathsf{M}_n)$ is a random point of $\mathbb{M}_1(\mathfrak{M})$. Let $\mathfrak{L}(\mathsf{M}_\infty) \in \mathbb{M}_1(\mathfrak{M})$ denote the law of the random map M_∞. It follows from [18, Thm. 4.1] that

$$\mathbb{P}((\mathsf{M}_n, v_n) \mid \mathsf{M}_n) \xrightarrow{p} \mathfrak{L}(\mathsf{M}_\infty). \tag{11}$$

The explicit construction of the limit M_∞ also entails that among the connected components created when removing any single vertex of M_∞ at most one is infinite. In particular,

$$\mathbb{P}(\mathsf{M}_\infty \in \Omega) = 1. \tag{12}$$

3.4 Proving Lemma 3 using the continuous mapping theorem

Let us recall the continuous mapping theorem (see, for example, the book by Billingsley [3, Thm. 2.7]) that says that random variables $X, X_1, X_2, \ldots$ that take values in a Polish space $\mathfrak{X}$ have the property that $X_n \xrightarrow{d} X$ implies $g(X_n) \xrightarrow{d} g(X)$, where $g : \mathfrak{X} \to \mathfrak{Y}$ is a measurable map to a Polish space $\mathfrak{Y}$ and X almost surely takes values on the subset of $\mathfrak{X}$, where g is continuous.

Hence, by combining the convergence (10) with Lemma 5 and Equation (12) allows us to apply the continuous mapping theorem with $\mathfrak{X} = \mathfrak{M}$ and $\mathfrak{Y} = \{0, 1\}$ to deduce

$$f(\mathsf{M}_n, v_n) \xrightarrow{d} f(\mathsf{M}_\infty).$$

In other words, the probability for v_n to be a cut vertex of M_n converges toward the probability $p = \mathbb{E}[f(\mathsf{M}_\infty)]$ that the root of M_∞ is a cut vertex. Equivalently, the number of vertices $\mathrm{v}(\mathsf{M}_n)$ in the map M_n satisfies

$$\mathbb{E}[X_n/\mathrm{v}(\mathsf{M}_n)] \to p.$$

Of course, it follows by the same arguments that in general for any sequence of probability measures $P_1, P_2, \ldots \in \mathbb{M}_1(\mathfrak{M})$ satisfying the weak convergence $P_n \Rightarrow \mathfrak{L}(\mathsf{M}_\infty)$, the push-forward measures satisfy

$$P_n f^{-1} \Rightarrow \mathfrak{L}(\mathsf{M}_\infty) f^{-1}. \tag{13}$$

Let us now consider the setting $\mathfrak{X} = \mathbb{M}_1(\mathfrak{M})$, $\mathfrak{Y} = \mathbb{R}$, and

$$g : \mathbb{M}_1(\mathfrak{M}) \to \mathbb{R}, \quad P \mapsto \int f \, \mathrm{d}P = P(f = 1). \tag{14}$$

That is, a probability measure $P \in \mathbb{M}_1(\mathfrak{M})$ gets mapped to the expectation of f with respect to P. In other words, to the P-probability that the root is a cut vertex. It follows from (13) that g is continuous at the point $\mathfrak{L}(\mathsf{M}_\infty)$. Hence, using (11) and again the continuous mapping theorem, it follows that

$$\mathbb{E}[f(\mathsf{M}_n, v_n) \mid \mathsf{M}_n] \xrightarrow{d} p. \tag{15}$$

As p is a constant, this convergence actually holds in probability. Moreover,

$$\mathbb{E}[f(\mathsf{M}_n, v_n) \mid \mathsf{M}_n] = X_n/\mathrm{v}(\mathsf{M}_n). \tag{16}$$

The number $\mathrm{v}(\mathsf{M}_n)$ is known to satisfy $\mathrm{v}(\mathsf{M}_n)/n \xrightarrow{p} 1/2$. In fact, a normal central limit theorem is known to hold (see, for example, [9, Lem. 4.1]). This allows us to apply Slutsky's theorem, yielding $X_n/n \xrightarrow{p} p/2$. We have thus completed the proof of Lemma 3.

3.5 Structural properties of the local limit

We let M denote a random map following a Boltzmann distribution with parameter $z_1 = \frac{1}{12}$. That is, M attains a finite planar map M with $\mathrm{c}(M)$ corners with probability

$$\mathbb{P}(\mathsf{M} = M) = \frac{z_1^{\mathrm{c}(M)}}{M(z_1)} = \frac{3}{4}\left(\frac{1}{12}\right)^{\mathrm{c}(M)}. \tag{17}$$

The local limit M_∞ exhibits a random number of independent copies of M close to its root. This can be made more precise by the following property.

▶ **Lemma 6.** *There is an infinite random planar map* M_∞^* *with a root vertex* u^* *that is not a cut vertex of* M_∞^**, such that* M_∞ *is distributed like the result of attaching an independent copy of* M *to each corner incident to* u^**.*

Here we use the term *attach* in the sense that the origin of the root-edge of the independent copy of M gets identified with the vertex u^*. In what follows we will only use the fact that such a (random) map M_∞^* exists. The proof of Lemma 6 (that is given in Appendix A) provides additional information about the distribution of M_∞ and M_∞^*.

3.6 Proving Lemma 4 via the asymptotic degree distribution

Let $q(z) = \sum_{k \geq 1} q_k z^k$ denote the probability generating function of the root-degree of the map M_∞^*. If we attach an independent copy of M to each corner incident to the vertex u^* in the map M_∞^*, then u^* becomes a cut vertex if and only if at least one of these copies has at least one edge. The probability for M to have no edges, that is, to consist only of a single vertex, is given by $1/M(z_1) = 3/4$. Hence the probability p for the root of M_∞ to be a cut vertex may be expressed by

$$p = \sum_{k \geq 1} q_k \left(1 - \left(\frac{3}{4}\right)^k\right) = 1 - q\left(\frac{3}{4}\right). \tag{18}$$

Hence, in order to determine p we need to determine $q(z)$. Surprisingly, we may do so without concerning ourselves with the precise construction of M_∞^*.

It was shown in [12] that the degree of the origin of the root-edge of the random planar map M_n admits a limiting distribution with a generating series $d(z)$ given by

$$d(z) = \frac{z\sqrt{3}}{\sqrt{(2+z)(6-5z)^3}}. \tag{19}$$

That is, $d_k := [z^k]d(z)$ is the asymptotic probability for the origin of the root-edge of M_n to have degree k. Let s_k denote the limit of the probability for a uniformly selected vertex of M_n to have degree k. It follows from [14, Prop. 2.6] that

$$s_k = 4d_k/k \tag{20}$$

for all integers $k \geq 1$. Setting $s(z) = \sum_{k \geq 1} s_k z^k$, Equation (20) may be rephrased by

$$zs'(z) = 4d(z). \tag{21}$$

Via integration, this yields the expression

$$s(z) = \frac{1}{2}\left(-1 + \frac{\sqrt{2+z}}{\sqrt{2 - \frac{5z}{3}}}\right) \tag{22}$$

As M_∞ is the local limit of M_n rooted at a uniformly chosen vertex, it follows that for each $k \geq 1$ the limit s_k equals the probability for the root of M_∞ to have degree k. Let $r(z)$ denote the probability generating series of the degree distribution of the origin of the root-edge of the Boltzmann map M. It follows from Lemma 6 that

$$s(z) = q(zr(z)). \tag{23}$$

We are going to compute $r(z)$. To this end, let $M(z,v)$ denote the generating series of planar maps with z marking edges and v marking the degree of the root vertex. By duality, $M(z,v)$ coincides with the bivariate generating series where the second variable marks the degree of the outer face. The quadratic method (see [11, p. 515] or compare with (1) and (2)) hence yields the known expression

$$M(z_1,u) = \frac{-3u^2+36u-36+\sqrt{3(u+2)(6-5u)^3}}{6u^2(u-1)}. \tag{24}$$

The series $r(z)$ is related to $M(z,u)$ via

$$r(u) = M(z_1,u)/M(z_1,1) = \frac{3}{4}M(z_1,u). \tag{25}$$

Forming the compositional inverse of $zr(z)$ and plugging it into Equation (23) yields the involved expression

$$q(z) = \frac{1}{2}\left(\frac{\sqrt{\frac{20z^2+48z-\sqrt{2z-27}(2z-3)^{3/2}+123}{z(4z+3)+24}}}{2\sqrt{\frac{6-4z}{-14z+5\sqrt{2z-27}\sqrt{2z-3}+51}}}-1\right). \tag{26}$$

Equation (26) allows us to evaluate the constant $q(3/4)$ in the expression for p given in Equation (18), yielding

$$p = 1-q(3/4) = \frac{5-\sqrt{17}}{2}. \tag{27}$$

This concludes the proof of Lemma 4.

4 A combinatorial approach to cut vertices of planar maps

The goal of this section is to re-derive the constant $(5-\sqrt{17})/4 = p/2$ in Theorem 1 with the help of a combinatorial approach by deriving an asymptotic expansion for the expected value $\mathbb{E}[X_n]$. We want to emphasize again that an extension of this approach (that will be given in the journal version of this paper) provides the asymptotic expansion of the second moment $\mathbb{E}[X_n^2]$ and consequently of the variance.

4.1 Generating function for the expected number of cut vertices

By extending the combinatorial approach that relates all planar maps with 2-connected maps (see (6)) it is possible to derive the following explicit formula for the generating function

$$E_a(z) = \sum_{n\ge 0} M_n \mathbb{E}[X_n] z^n.$$

▶ **Lemma 7.** *Let $u_1(z)$ denote the function $u_1(z) = 1/(1-V(z,1)$, where $V(z,x)$ (and $U(z,x)$) is given by (5). Then we have*

$$\begin{aligned} E_a(z) = &\frac{1}{1-2zM(z)A_z(zM(z)^2,1,1)} \\ &\times\Big[A(zM(z)^2,1,1)+A_x(zM(z)^2,1,1) \\ &\quad -2zM(z)-z-B(zM(z)^2,1,1/M(z))-B^\bullet(zM(z)^2,1/M(z)) \\ &\quad +2zM(z)A_z(zM(z)^2,1,1)\left(B(zM(z)^2,1,1/M(z))-M(z)+zM(z)+z+1\right)\Big], \end{aligned} \tag{28}$$

where

$$B^\bullet(z,w) = zw\frac{\frac{u_1(z)B(z,1,w)-wB(z,1,u_1(z))}{w-u_1(z)} + zwu_1(z)}{1-\frac{u_1(z)B(z,1,w)-wB(z,1,u_1(z))}{w-u_1(z)} - zwu_1(z)}. \tag{29}$$

The proof is given in Appendix B. Note that all involved functions are algebraic, which shows that the generating function $E_a(z)$ is algebraic, too.

4.2 Asymptotics

We start with a proper representation of $B_x(z,1,1)$ and $B_z(z,1,1)$.

▶ **Lemma 8.** *Let $B(z,x,u)$ be given by (4) and $u_1(z) = 1/(1-V(z,1))$ as in Lemma 11. Then we have*

$$B_x(z,1,1) = \frac{u_1(z)-1}{u_1(z)}Q(z)(1-Q(z)) \tag{30}$$

and

$$B_z(z,1,1) = \frac{u_1(z)-1}{z\,u_1(z)}Q(z)(1-Q(z)) + u_1(z) - 1 \tag{31}$$

where $Q(z)$ abbreviates

$$Q(z) = \frac{V(z,1)^2}{u_1(z)-1} - \frac{u_1(z)B(z,1,1)}{u_1(z)-1} + z\,u_1(z).$$

The proof is an easy application of the kernel method applied to the derivative of the defining relation (3).

▶ **Lemma 9.** *We have the following local expansions in powers of $\left(1-\frac{27}{4}z\right)$:*

$$B_x(z,1,1) = \frac{2}{27} - \frac{2\sqrt{3}}{27}\sqrt{1-\frac{27}{4}z} + \frac{2}{81}\left(1-\frac{27}{4}z\right) + \frac{19\sqrt{3}}{729}\left(1-\frac{27}{4}z\right)^{3/2} + \cdots \tag{32}$$

$$B_z(z,1,1) = 1 - \sqrt{3}\left(1-\frac{27}{4}z\right)^{1/2} + \frac{4}{3}\left(1-\frac{27}{4}z\right) - \frac{35\sqrt{3}}{54}\left(1-\frac{27}{4}z\right)^{3/2} + \cdots \tag{33}$$

$$\begin{aligned} B^\bullet(z,w) = {} & -4\,\frac{w\left(-2\,w+\sqrt{4\,w^2-60\,w+81}-9\right)}{243-54\,w+27\,\sqrt{4\,w^2-60\,w+81}} \\ & + \frac{16\,\sqrt{3}w^2\left(-2\,w+\sqrt{4\,w^2-60\,w+81}+3\right)}{9\left(9-2\,w+\sqrt{4\,w^2-60\,w+81}\right)^2(2\,w-3)}\sqrt{1-\frac{27}{4}z} + \cdots \end{aligned} \tag{34}$$

Proof. By inverting the equation $z = V(1-V)^2$ it follows that $V(z,1)$ has the local expansion

$$V(z,1) = \frac{1}{3} - \frac{2}{3\sqrt{3}}Z + \frac{2}{27}Z^2 - \frac{5}{81\sqrt{3}}Z^3 + \cdots,$$

where Z abbreviates

$$Z = \sqrt{1-\frac{27}{4}z}.$$

Consequently $u_1(z) = 1/(1-V(z,1))$ is given by

$$u_1(z) = \frac{3}{2} - \frac{\sqrt{3}}{2}Z + \frac{2}{3}Z^2 - \frac{35\sqrt{3}}{108}Z^3 \cdots$$

We already know that

$$B(z,1,u_1(z)) = V(z,1)^2 = \frac{1}{9} - \frac{4\sqrt{3}}{27}Z + \frac{16}{81}Z^2 - \frac{34\sqrt{3}}{729}Z^3 + \cdots$$

and from (4) we directly obtain

$$B(z,1,1) = \frac{1}{27} - \frac{4}{27}Z^2 + \frac{8\sqrt{3}}{81}Z^3 + \cdots$$

Hence, the local expansion of $Q(z) = Q_0(z,1,u_1(z))$ can be easily calculated:

$$Q(z) = \frac{1}{3} - \frac{2\sqrt{3}}{9}Z + \frac{2}{27}Z^2 - \frac{5\sqrt{3}}{243}Z^3 + \cdots,$$

and, thus, (32) and (33) follow from this expansion and from (30) and (31).

Finally we have to use (29) and the expansion for $B(x,1,w)$ to obtain (34). ◀

This leads us to the following local expansion for $E_a(z)$ and a corresponding asymptotic relation.

▶ **Lemma 10.** *The function $E_a(z)$ has the following local expansion*

$$E_a(z) = \frac{11\sqrt{17}-37}{24} - (5-\sqrt{17})\sqrt{1-12z} + \cdots \tag{35}$$

which implies

$$\mathbb{E}[X_n] = \frac{[z^n]\, E_a(z)}{[z^n]\, M(z)} = \frac{(5-\sqrt{17})}{4}n + O(1).$$

Proof. We note that several parts of (28) have a dominant singulartiy of the form $(1-12z)^{3/2}$. For those parts only the value at $z_1 = 1/12$ influences the constant term and coefficient of $\sqrt{1-12z}$ in the local expansion of $E_a(z)$. In particular we have

$$\begin{aligned} M(z_1) &= \frac{4}{3}, \\ A(z_1M(z_1)^2,1,1) &= \frac{1}{3}, \\ B(z_1M(z_1)^2,1,1/M(z_1)) &= \frac{3\sqrt{17}-11}{72}. \end{aligned}$$

The other appearing function will have a non-zero coefficient at the $\sqrt{1-12z}$–term. Note also that we have

$$\sqrt{1-\frac{27}{4}zM(z)^2} = \sqrt{3}\sqrt{1-12z} - \frac{2}{3}\sqrt{3}(1-12z) + O((1-12z)^{3/2}).$$

Hence we get

$$\begin{aligned} A_z(zM(z)^2,1,1) &= 3 - 3\sqrt{1-12z} + \cdots, \\ A_x(zM(z)^2,1,1) &= \frac{2}{9} - \frac{2}{9}\sqrt{1-12z} + \cdots, \\ B^\bullet(zM(z)^2,1,1,1/M(z)) &= \frac{\left(7-\sqrt{17}\right)\left(5-\sqrt{17}\right)}{72} - \frac{\left(1+\sqrt{17}\right)\left(-5+\sqrt{17}\right)^2}{48}\sqrt{1-12z} + \cdots \end{aligned}$$

and so (35) follows.

From (35) it directly follows that

$$[z^n]\, E_a(z) = \frac{5-\sqrt{17}}{2\sqrt{\pi}}n^{-3/2}12^n \cdot (1+O(1/n))$$

By dividing that by $M_n = [z^n]M(z) = (2/\sqrt{\pi})n^{-5/2}12^n \cdot (1+O(1/n))$ the final result follows. ◀

5 Outerplanar Maps

We give a proof of Theorem 2 for the case of (all) outerplanar maps. (The proof in the bipartite case is very similiar.)

We recall that the generating function $M_O(z)$ of outerplanar maps satisfies (7), where the function

$$A_O(z) = \frac{1}{4}\left(1 + z - \sqrt{1 - 6z + z^2}\right)$$

is the generating function for polygon dissections (plus a single edge) has radius of convergence $z_{0,O} = 3 - 2\sqrt{2}$. From this we obtain

$$M_O(z) = \frac{z\left(3 - \sqrt{1 - 8z}\right)}{2(1 + z)}.$$

The radius of convergence of $M_O(z)$ is $z_{1,O} = \frac{1}{8}$ so that $M_O(z_{1,O}) = \frac{1}{18} < z_{0,O}$. Note that $M_O(z)$ has a squareroot singularity (as it has to be). Now let $M_O(z, y)$ denote the generating function of outerplanar maps, where y takes care of the number of cut-vertices. We already mentioned that $M_O(z, y)$ satisfies the functional equation

$$M_O(z, y) = \frac{z}{1 - A_O(z + y(M_O(z, y) - z))}$$

which gives

$$M_O(z, y) = \frac{z\left(3 - z + yz - \sqrt{(y - 1)z^2 - (6 + 2y)z + 1}\right)}{2(1 + yz)}.$$

Clearly, if y is sufficiently close to 1 then the singularities of $M_O(z, y)$ and $A_O(z)$ do not interact and so we obtain a squareroot singularity

$$\rho(y) = \frac{3 + y - 2\sqrt{2 + 2y}}{(y - 1)^2}.$$

for the mapping $z \mapsto M_O(z, y)$. Note that $\rho(y)$ is actually regular at $y = 1$ and satisfies $\rho(1) = 1/8$.

By [7, Theorem 2.25] we immediately obtain a central limit theorem with $\mathbb{E}[X_n] = c\,n + O(1)$ and variance $\mathbb{V}\mathrm{ar}[X_n] = \sigma^2 n + O(1)$, where

$$c = -\frac{\rho'(1)}{\rho(1)} = \frac{1}{4} \quad \text{and} \quad \sigma^2 = -\frac{\rho''(1)}{\rho(1)} + \mu + \mu^2 = \frac{5}{32}.$$

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A Proof of Lemma 6

A direct description of the limit M_∞ that uses a generalization of the Bouttier, Di Francesco and Guitter bijection [5] was given in [18, Thm. 4.1]. Although the structure of M_∞ may be studied in this way, it will be easier to show that M_∞ has the desired shape via a construction related to limits of the 2-connected core within M_n.

Let $\mathcal{B}(\mathsf{M}_n) \subset \mathsf{M}_n$ denote the largest (meaning, having a maximal number of edges) 2-connected block in the map M_n. Typically $\mathcal{B}(\mathsf{M}_n)$ is uniquely determined, as the number $c(n)$ of corners of $\mathcal{B}(\mathsf{M}_n)$ is known to have order $2n/3$, and the number of corners in the second largest block has order $n^{2/3}$.

Consider the random planar map $\bar{\mathsf{M}}_n$ constructed from the core $\mathsf{C}_n := \mathcal{B}(\mathsf{M}_n)$ by attaching for each integer $1 \le i \le c(n)$ an independent copy $\mathsf{M}(i)$ of M at the ith corner of C_n. We use the notation C_n instead of $\mathcal{B}(\mathsf{M}_n)$ from now on to emphasize that we consider C_n always as a part of $\bar{\mathsf{M}}_n$ (as opposed to M_n).

Clearly, the two models M_n and $\bar{\mathsf{M}}_n$ are not identically distributed. For example, the number of edges in $\bar{\mathsf{M}}_n$ is a random quantity that fluctuates around n. However, analogously as in the proof of [17, Lem. 9.2], local convergence of $\bar{\mathsf{M}}_n$ is equivalent to local convergence of M_n, implying that M_∞ is also the local limit of $\bar{\mathsf{M}}_n$ with respect to a uniformly selected vertex u_n.

The random 2-connected planar map B_n with n edges was shown to admit a local limit $\hat{\mathsf{B}}$ that describes the asymptotic vicinity of a typical corner (equivalently, the root-edge of B_n), see [17, Thm. 1.3]. Arguing entirely analogously as in [9], it follows that there is also a local limit B_∞ that describes the asymptotic vicinity of a typical vertex.

The number of vertices of $\bar{\mathsf{M}}_n$ has order $n/2$, and the number of vertices in C_n is known to have order $n/6$. Let u_n^{B} denote the result of conditioning the random vertex u_n to belong to C_n. The probability for this to happen tends to $1/3$. As u_n^{B} is uniformly distributed among all vertices of C_n, it follows that $(\mathsf{C}_n, u_n^{\mathrm{B}}) \xrightarrow{d} \mathsf{B}_\infty$ in the local topology. This implies that $(\bar{\mathsf{M}}_n, u_n^{\mathrm{B}})$ converges in distribution towards the result $\mathsf{M}_\infty^{\mathrm{B}}$ of attaching an independent copy of M to each corner of B_∞. The limit $\mathsf{M}_\infty^{\mathrm{B}}$ has the desired shape.

Let u_n^{c} denote the result of conditioning the random vertex u_n to lie outside of C_n. It remains to show that the limit $\mathsf{M}_\infty^{\mathrm{c}}$ of $(\bar{\mathsf{M}}_n, u_n^{\mathrm{c}})$ has the desired shape as well. Let $1 \le i_n \le c(n)$ denote the index of the corner where the component containing u_n^{c} is attached. It is important to note that given the maps $\mathsf{M}(1), \ldots, \mathsf{M}(c(n))$, the random integer i_n need not be uniform, as it is more likely to correspond to a map with an above average number of vertices. This well-known waiting time paradox implies that *asymptotically* the component containing u_n^{c} follows a size-biased distribution $\mathsf{M}^\bullet$. That is, $\mathsf{M}^\bullet$ is a random finite planar map with a marked non-root vertex, such that for any planar map M with a marked non-root vertex v it holds that

$$\mathbb{P}(\mathsf{M}^\bullet = (M, v)) = \mathbb{P}(\mathsf{M} = M)/(\mathbb{E}[\mathrm{v}(\mathsf{M})] - 1),$$

with $\mathrm{v}(\mathsf{M})$ denoting the number of vertices in the Boltzmann planar map M.

In detail: Given the random number $c(n)$, let i_n^* be uniformly selected among the integers from 1 to $c(n)$. For each $1 \le i \le c(n)$ with $i \ne i_n^*$ let $\bar{\mathsf{M}}(i)$ denote an independent copy of M, and let $\bar{\mathsf{M}}(i_n^*)$ denote an independent copy of $\mathsf{M}^\bullet$. Likewise, for each $1 \le i \le c(n)$ with $i \ne i_n$ set $\mathsf{M}^*(i) = \mathsf{M}(i)$, and let $\mathsf{M}^*(i_n) = (\mathsf{M}(i_n), u_n^{\mathrm{c}})$. Analogously as in the proof of [17, Lem. 9.2], it follows that

$$(\mathsf{M}^*(i))_{1 \le i \le c(n)} \overset{d}{\approx} (\bar{\mathsf{M}}(i))_{1 \le i \le c(n)}.$$

This entails that the core C_n rooted at the corner with index i_n admits $\hat{\mathsf{B}}$ (and not B_∞) as local limit. Moreover, the local limit $\mathsf{M}_\infty^{\mathrm{c}}$ of $\bar{\mathsf{M}}_n$ rooted at u_n^{c} may be constructed by attaching an independent copy of M to each corner of $\hat{\mathsf{B}}$, except for the root-corner of $\hat{\mathsf{B}}$, which receives an independent copy of $\mathsf{M}^\bullet$. The marked vertex of the limit object $\mathsf{M}_\infty^{\mathrm{c}}$ is then given by the marked vertex of this component.

To proceed, we need information on the shape of $\mathsf{M}^\bullet$. Consider the ordinary generating functions $M(v, w)$ and $A(v, w)$ of planar maps and 2-connected planar maps, with v marking corners, and w marking non-root vertices. The block-decomposition yields

$$M(v, w) = A(vM(v, w), w). \tag{36}$$

That is, a planar map consists of a uniquely determined block containing the root-edge, with uniquely determined components attached to each of its corners. Let us call this block the *root block*. For the trivial map consisting of a single vertex and no edges, this block is identical to the trivial map, with nothing attached to it as it has no corners.

Marking a non-root vertex (and no longer counting it) corresponds to taking the partial derivative with respect to w. It follows from (36) that

$$\frac{\partial M}{\partial w}(v, w) = \frac{\partial A}{\partial w}(vM(v, w), w) + \frac{\partial A}{\partial v}(vM(v, w), w) v \frac{\partial M}{\partial w}(v, w).$$

The combinatorial interpretation is that either the marked non-root vertex is part of the root block (accounting for the first summand), or there is a uniquely determined corner of the root block such that the component attached to this corner contains it. This is a recursive decomposition, as in the second case we could proceed with this component, considering whether the marked vertex belongs to its root block or not. We may do so a finite number of times, until it finally happens that the marked vertex belongs to the root-block of the component under consideration. That is, if we follow this decomposition until encountering the marked non-root vertex, we have to pass through a uniquely determined sequence of blocks, always proceeding along uniquely determined (and hence marked) corners, until arriving at a block with a marked non-root vertex. On a generating function level, this is expressed by

$$\frac{\partial M}{\partial w}(v,w) = \frac{1}{1-\frac{\partial A}{\partial v}(vM(v,w),w)v}\frac{\partial A}{\partial w}(vM(v,w),w).$$

This allows us to apply Boltzmann principles, yielding that the random map $\mathsf{M}^\bullet$ may be sampled in two steps, that may be described as follows: First, generate this sequence of blocks by linking a geometrically distributed random number N of random independent Boltzmann distributed blocks $\mathsf{B}_1^\circ,\dots,\mathsf{B}_N^\circ$ with marked corners into a chain, and attach an extra random Boltzmann distributed block $\mathsf{B}^\bullet$ with a marked non-root vertex to the end of the chain. The random number N has generating function

$$\mathbb{E}[u^N] = \frac{1-\frac{\partial A}{\partial v}(z_1M(z_1,1),1)z_1}{1-u\frac{\partial A}{\partial v}(z_1M(z_1,1),1)z_1}.$$

The corner-rooted blocks are independent copies of a Boltzmann distributed block B°, whose number of corners $\mathrm{c}(\mathsf{B}^\circ)$ has generating function

$$\mathbb{E}[u^{\mathrm{c}(\mathsf{B}^\circ)}] = \frac{\frac{\partial A}{\partial v}(uz_1M(z_1,1),1)}{\frac{\partial A}{\partial v}(z_1M(z_1,1),1)}.$$

The distribution of B° is fully characterized by the fact that, when conditioning on the number of corners, B° is conditionally uniformly distributed among the corner-rooted blocks with that number of corners. The distribution of $\mathsf{B}^\bullet$ is defined analogously. If we attach a block $\tilde{B}$ to the marked corner c of some block B, we say the resulting corner "to the right" of $\tilde{B}$ *corresponds* to c. Hence the map obtained by linking $(\mathsf{B}_1^\circ,\dots,\mathsf{B}_N^\circ,\mathsf{B}^\bullet)$ has precisely N corners that correspond to marked corners. We call these corners *closed*, and all other corners *open*. The second and final step in the sampling procedure of $\mathsf{M}^\bullet$ is to attach an independent copy of M to each open corner of the map corresponding to $(\mathsf{B}_1^\circ,\dots,\mathsf{B}_N^\circ,\mathsf{B}^\bullet)$. Note that since the marked vertex of $\mathsf{B}^\bullet$ is a non-root vertex, all corners incident to the marked vertex are open. Consequently, the limit $\mathsf{M}_\infty^{\mathrm{c}}$ has the desired shape, and the proof is complete.

B Proof of Lemma 7

First we introduce (formally) a generating function that takes care of all vertex degrees in 2-connected planar maps (including the one-edge map and the one-edge loop)

$$\overline{A}(z;w_1,w_2,w_3,w_4,\dots;u),$$

where w_k, $k\ge 1$, corresponds to vertices of degree k and we also take the root vertex into account. As usual, u corresponds to the root degree.

Similarly we introduce a variant of this generating function that takes care of all vertex degrees in 2-connected planar maps (without the one-edge map and one-edge loop) and does not take the root vertex into account:

$$\overline{B}(z; w_2, w_3, w_4, \ldots; u).$$

It seems to be impossible to work directly with $\overline{A}(z; w_1, w_2, w_3, \ldots)$ or with $\overline{B}(z; w_2, w_3, w_4, \ldots; u)$, however, we have the following easy relations:

$$\overline{A}(z; xv, xv^2, xv^3, \ldots; u) = xA(zv^2, x, u), \ \overline{B}(z; xv^2, xv^3, \ldots; u) = B(zv^2, x, u/v).$$

This follows from the fact that every vertex of degree k corresponds to k half-edges. So summing up these half-edges we get twice the number of edges. In particular by taking derivatives with respect to x and v it follows that

$$\sum_{k\ge 1} \overline{A}_{w_k}(z; v, v^2, v^3, \ldots)v^k = A(zv^2, 1, 1) + A_x(zv^2, 1, 1) \tag{37}$$

and

$$\sum_{k\ge 1} k\overline{A}_{w_k}(z; v, v^2, v^3, \ldots)v^{k-1} = 2zvA_z(zv^2, 1, 1). \tag{38}$$

It turns out that we will also have to deal with the sum of all derivatives which is slightly more difficult to understand.

▶ **Lemma 11.** *Let $u_1(z)$ denote the function $u_1(z) = 1/(1 - V(z, 1)$, where $V(z, x)$ (and $U(z, x)$) is given by (5). Then we have*

$$\sum_{k\ge 1} \overline{A}_{w_k}(z; v, v^2, v^3, \ldots) = 2zv + z + B(zv^2, 1, 1/v) \tag{39}$$

$$+ zv \frac{\frac{u_1(zv^2)B(zv^2,1,1/v) - B(zv^2,1,u_1(zv^2))/v}{1/v - u_1(zv^2)} + zvu_1(zv^2)}{1 - \frac{u_1(zv^2)B(zv^2,1,1/v) - B(zv^2,1,u_1(zv^2))/v}{1/v - u_1(zv^2)} - zvu_1(zv^2)}$$

Proof. We note that the derivative with respect to w_k marks a vertex of degree k and discounts it. By substituting w_k by v^k we, thus, see that the resulting exponent of v is twice the number of edges minus the degree of the marked vertex. Hence we have to cover the situation, where we mark a vertex and keep track of the degree of the marked vertex.

Let $B^\bullet(z, x, u, w)$ be the generating function of vertex marked 2-connected planar maps, where the marked vertex is different from the root and where u takes care of the root degree and w of the degree of the pointed vertex. By duality this is also the generating function of face marked 2-connected planar maps where u takes care of the root face valency and w of the valency of the marked face (that is different from the root face). Then we have

$$\sum_{k\ge 1} \overline{A}_{w_k}(z; v, v^2, v^3, \ldots) = 2zv + z + B(zv^2, 1, 1/v) + B^\bullet(zv^2, 1, 1, 1/v).$$

The term $2zv$ corresponds to the one-edge map, the term z to the one-edge loop, the term $B(zv^2, 1/v)$ to the case where the root vertex is marked and the third term $B^\bullet(zv^2, 1, 1, 1/v)$ to the case where a vertex different from the root is marked. Note that the substitution $u = 1/v$ (or $w = 1/v$) discounts the degree of the marked vertex in the exponent of v as needed.

Thus, it remains to get an expression for $B^\bullet(z,1,u,w)$. For this purpose we start with the generating function $B(z,1,u)$ and determine first the generating function $\tilde{B}(z,x,u,w)$ (for $x=1$), where the additional variable w takes care of the valency of the second face incident to the root edge. By using the same construction as above we have

$$\tilde{B}(z,1,u,w) = zuw\frac{\frac{uB(z,1,w)-wB(z,1,u)}{w-u} + zuw}{1-\frac{uB(z,1,w)-wB(z,1,u)}{w-u} - zuw}.$$

This gives (by again applying this construction)

$$B^\bullet(z,1,u,w) = \tilde{B}(z,1,u,w) + zu\frac{\frac{uB^\bullet(z,1,1,w)-B^\bullet(z,1,u,w)}{1-u}}{\left(1-\frac{uB(z,1,1)-B(z,1,u)}{1-u} - zu\right)^2}.$$

This equation can be solved with the help of the kernel method. By rewriting it to

$$B^\bullet(z,1,u,w)\left(1+\frac{zu}{1-u}\frac{1}{\left(1-\frac{uB(z,1,1)-B(z,1,u)}{1-u}-zu\right)^2}\right)$$
$$= B(z,1,u,w) + \frac{zu^2B^\bullet(z,1,1,w)}{1-u}\frac{1}{\left(1-\frac{uB(z,1,1)-B(z,1,u)}{1-u}-zu\right)^2}$$

we observe that by setting $u_1(z) = 1/(1-V(z,1))$ the left hand side cancels. This implies

$$B(z,1,u_1(z),w) + \frac{zu_1(z)^2B^\bullet(z,1,1,w)}{1-u_1(z)}\frac{1}{\left(1-\frac{u_1(z)B(z,1,1)-B(z,1,u_1(z))}{1-u_1(z)}-zu_1(z)\right)^2} = 0$$

and leads (after some simple algebra) finally to (39). ◀

Let $M_0(z,y)$ denote the generating function of planar maps with at least one edge, where the root vertex is not a cut point and where z takes care of the number of edges and y of the number of cut-points (that are then different from the root vertex). Next let $M_r(z,y)$ denote the generating function of (all) planar maps, where z takes care of the number of edges and y of the number of non-root cut-points. Finally let $M_a(z,y)$ denote the generating function of (all) planar maps, where z takes care of the number of edges and y of the number of (all) cut-points. Obviously we have the following relation between these three generating functions:

$$M_a(z,y) = yM_r(z,y) - (y-1)(1+M_0(z,y)). \tag{40}$$

Note that $M_0(z,1) = \overline{B}\left(z;M(z)^2,M(z)^3,\ldots;1\right) = B(zM(z)^2,1,1/M(z)) + zM(z) + z$.

Furthermore we set

$$E_a(z) = \left.\frac{\partial M_a(z,y)}{\partial y}\right|_{y=1} = \sum_{n\ge 0} M_n\mathbb{E}[X_n]z^n \quad \text{and} \quad E_r(z) = \left.\frac{\partial M_r(z,y)}{\partial y}\right|_{y=1}.$$

By differentiating (40) with respect to y and setting $y=1$ we obtain

$$E_a(z) = E_r(z) + M(z) - 1 - M_0(z,1). \tag{41}$$

With the help of the above notions we obtain the following (formal relation):

$$M_a(z,y) = 1 + \overline{A}\left(z; yM_r(z,y)-y+1, yM_r(z,y)^2-y+1,\ldots;1\right). \tag{42}$$

The right hand side is based on the block-decompostion (similarly to (6)) and takes care whether the vertices of the block that contains the root edge become cut-vertices or not. By differentiating (42) with respect to y and setting $y = 1$ we, thus, obtain

$$\begin{aligned} E_a(z) &= \sum_{k\ge 1} \overline{A}_{w_k}\left(z; M(z), M(z)^2, \ldots; 1\right)\left(M(z)^k - 1 + kM(z)^{k-1}E_r(z)\right) \\ &= \sum_{k\ge 1} \overline{A}_{w_k}\left(z; M(z), M(z)^2, \ldots\right) M(z)^k - \sum_{k\ge 1} \overline{A}_{w_k}\left(z; M(z), M(z)^2, \ldots\right) \\ &+ E_r(z) \sum_{k\ge 1} k\overline{A}_{w_k}\left(z; M(z), M(z)^2, \ldots\right) M(z)^{k-1}. \end{aligned}$$

By using (41) we get a proper expression for $E_a(z)$. At this stage we can apply (37) and (38) with $v = M(z)$. Furthermore Lemma 11 gives

$$\begin{aligned} &\sum_{k\ge 1} \overline{A}_{w_k}(z; M(z), M(z)^2, \ldots) \\ &= 2zM(z) + z + B(zM(z)^2, 1, 1/M(z)) + B^\bullet(zM(z)^2, 1, 1, 1/M(z)) \\ &= 2zM(z) + z + B(zM(z)^2, 1, 1/M(z)) \\ &+ zM(z) \frac{\frac{u_1(zM(z)^2)B(zM(z)^2,1,1/M(z)) - B(zM(z)^2,1,u_1(zM(z)^2))/M/z)}{1/M(z) - u_1(zM(z)^2)} + zM(z)u_1(zM(z)^2)}{1 - \frac{u_1(zM(z)^2)B(zM(z)^2,1,1/M(z)) - B(zM(z)^2,1,u_1(zM(z)^2))/M(z)}{1/M(z) - u_1(zM(z)^2)} - zM(z)u_1(zM(z)^2)} \end{aligned}$$

This finally leads to the proposed explicit formula for $E_a(z)$.

Asymptotics of Minimal Deterministic Finite Automata Recognizing a Finite Binary Language

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Abstract

We show that the number of minimal deterministic finite automata with $n+1$ states recognizing a finite binary language grows asymptotically for $n \to \infty$ like

$$\Theta\left(n!\, 8^n e^{3a_1 n^{1/3}} n^{7/8}\right),$$

where $a_1 \approx -2.338$ is the largest root of the Airy function. For this purpose, we use a new asymptotic enumeration method proposed by the same authors in a recent preprint (2019). We first derive a new two-parameter recurrence relation for the number of such automata up to a given size. Using this result, we prove by induction tight bounds that are sufficiently accurate for large n to determine the asymptotic form using adapted Netwon polygons.

2012 ACM Subject Classification Theory of computation → Regular languages; Mathematics of computing → Enumeration; Mathematics of computing → Generating functions

Keywords and phrases Airy function, asymptotics, directed acyclic graphs, Dyck paths, bijection, stretched exponential, compacted trees, minimal automata, finite languages

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.11

Related Version The companion paper "Compacted binary trees admit a stretched exponential" by the same authors is available at arXiv:1908.11181.

Funding *Andrew Elvey Price*: European Research Council (ERC) in the European Union's Horizon 2020 research and innovation programme, under the Grant Agreement No. 759702.
Wenjie Fang: *Recherche en esprit libre*, *i.e.*, not supported by fundings with precise predefined goals.
Michael Wallner: Erwin Schrödinger Fellowship of the Austrian Science Fund (FWF): J 4162-N35.

Acknowledgements We would like to thank Cyril Banderier, Tony Guttmann, and Andrea Sportiello for interesting discussions on the presence of a stretched exponential. We also thank our referees for their careful reading and helpful comments.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 11; pp. 11:1–11:13
Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

1 Introduction

A *deterministic finite automaton* (DFA) A is a 5-tuple $(\Sigma, Q, \delta, q_0, F)$, where Σ is a finite set of letters called the *alphabet*, Q is a finite set of states, $\delta : Q \times \Sigma \to Q$ is the *transition function*, q_0 is the *initial state*, and $F \subseteq Q$ is the set of *final states* (sometimes called *accept states*). States not in F are called *non-final* or *reject states*. A DFA can be represented by a directed graph with one vertex v_s for each state $s \in Q$, with the vertices corresponding to final states being highlighted, and for every transition $\delta(s, w) = \hat{s}$, there is an edge from s to $\hat{s}$ labeled w (see Figure 1).

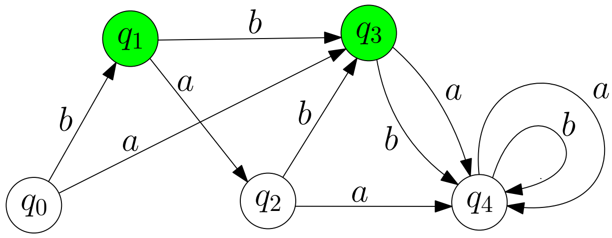


Figure 1 The unique minimal DFA for the language $\{a, b, bab, bb\}$. Here, q_0 is the initial state, q_1 and q_3 are the final states, and q_4 is the unique sink.

A word $w = w_1 w_2 \cdots w_\ell \in \Sigma^*$ is *accepted* by A if the sequence of states $(s_0, s_1, \ldots, s_\ell) \in Q^{\ell+1}$ defined by $s_0 = q_0$ and $s_{i+1} = \delta(s_i, w_i)$ for $i = 0, \ldots, \ell - 1$ ends with $s_\ell \in F$ a final state. The set of words accepted by A is called the *language* $\mathcal{L}(A)$ recognized by A. It is well-known that DFAs recognize exactly the set of regular languages. Note that every DFA recognizes a unique language, but a language can be recognized by several different DFAs. A DFA is called *minimal* if no DFA with fewer states recognizes the same language. The Myhill-Nerode Theorem states that every regular language is recognized by a unique minimal DFA (up to isomorphism) [8, Theorem 3.10]. For more details on automata see [8].

In this paper we show that the counting sequence $(m_{2,n})_{n\in\mathbb{N}}$ of minimal DFAs of size n recognizing a finite binary language admits a stretched exponential. Until now, the problem of counting these automata, even asymptotically, was widely open, see for example [4].

▶ **Theorem 1.** *The number $m_{2,n}$ of non-isomorphic minimal DFAs on a binary alphabet recognizing a finite language with $n + 1$ states satisfies for $n \to \infty$*

$$m_{2,n} = \Theta\left(n!\, 8^n e^{3a_1 n^{1/3}} n^{7/8}\right),$$

where $a_1 \approx -2.338$ is the largest root of the Airy function.

Since every regular language defines a unique minimal automaton, one may define the (space) complexity of the language to be the number of states in this corresponding automaton. Defining *space complexity* in this way, the number $m_{2,n}$ is simply the number of finite languages over a binary alphabet of space complexity $n + 1$.

In the recent paper [6] we showed lower and upper asymptotic bounds on $m_{2,n}$ by first establishing a connection between automata counted by $m_{2,n}$ and classes of directed acyclic graphs (DAGs) and then solving their asymptotic enumeration problem. In particular, we proved that

$$2^{n-1} c_n \le m_{2,n} \le 2^{n-1} r_n, \tag{1}$$

where c_n is the number of compacted and r_n the number of relaxed binary trees of size n. These appear naturally in the compression of XML documents [3, 7]. In the same paper, we showed that as $n \to \infty$,

$$c_n = \Theta\left(n!\, 4^n e^{3a_1 n^{1/3}} n^{3/4}\right) \qquad \text{and} \qquad r_n = \Theta\left(n!\, 4^n e^{3a_1 n^{1/3}} n\right),$$

leading to asymptotic lower and upper bounds on $m_{2,n}$. The results of the present work arise as a further application of the general method from [6] for proving the appearance of such stretched exponentials. They showcase the strength of our method, and we expect that our method may be applied to yet other combinatorial objects governed by similar recurrences.

The asymptotic proportion of general minimal DFAs (not necessarily recognizing a *finite* language) was solved by Bassino, Nicaud, and Sportiello in [1], building on enumeration results by Korshunov [9, 10] and Bassino and Nicaud [2]. The result in [1] also exploits an underlying tree structure of the related automata, but from a different traversal than what we use. In that case, no stretched exponential appears in the asymptotic enumeration, and the minimal automata account for a constant fraction of all automata.

2 Recurrence relation

To derive a recurrence for automata recognizing a finite language, we need the following lemma. In the following, we only consider automata on the binary alphabet $\{a, b\}$.

▶ **Lemma 2** ([11, Lemma 2.3], [8, Section 3.4])**.** *A DFA A is the minimal automaton for some finite language if and only if it has the following properties:*

- **(a)** *There is a unique* sink s. *That is, a state which is not a final state such that all transitions from s end at s that is, $\delta(s, w) = s$.*
- **(b)** *A is* acyclic*: the underlying directed graph has no cycles except for the loops at the sink.*
- **(c)** *A is* initially connected*: for any state p there exists a word $w \in \Sigma^*$ such that A reaches the state p upon reading w.*
- **(d)** *A is* reduced*: for any two different states q, q', the two automata with initial state q and q' recognize different languages.*

Next, we identify a property that can replace the one of being *reduced*.

▶ **Lemma 3.** *An acyclic, initially connected DFA A with a unique sink is reduced if and only if it satisfies the following condition:*

- **(d')** State uniqueness: *there are no two distinct states q and q' with $\delta(q, a) = \delta(q', a)$ and $\delta(q, b) = \delta(q', b)$ such that both q and q', or neither q nor q', are accept states.*

Proof. By definition, being reduced implies state uniqueness. Now suppose that A is not reduced while state uniqueness holds. Then there are two states $q \neq q'$ in A such that the two automata with initial state q and q' recognize the same language L. As A is acyclic, L is finite. We define the weight of L to be $\sum_{w \in L}(|w| + 1)$, and we pick q, q' such that the weight of L is minimal.

Suppose that L is not empty. By the state uniqueness, we must have $\delta(q, a) \neq \delta(q', a)$ or $\delta(q, b) \neq \delta(q', b)$. Without loss of generality, suppose that $r = \delta(q, a) \neq \delta(q', a) = r'$. The two automata with initial state r and r' recognize the same language $a^{-1}L = \{w \mid aw \in L\}$. Since the weights of $a^{-1}L$ are strictly less that that of L, we have r and r' violating the minimality of the weight of L. Therefore, L must be empty.

Since L is empty, q and q' are both rejecting. They cannot both be the sink as the sink is unique. Suppose that q is not the sink. Then due to state uniqueness, among $\delta(q, a)$ and $\delta(q, b)$ there is at least one state q_1 that is not the sink. As L is empty, q_1 is also rejecting.

We can then replace q with q_1 and perform the same argument to q_1 and q', repeating *ad infinitum*. This creates an infinite sequence of states without repetition since A is acyclic. This is impossible as A is a DFA. Therefore, the existence of q and q' is impossible, meaning that A is reduced. We thus have the desired equivalence. ◀

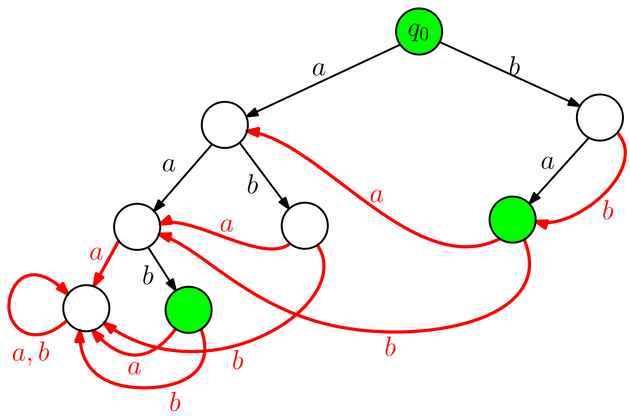


Figure 2 An acyclic DFA with its spanning subtree in black and all other edges in red. The initial state is q_0 and the finial states are colored green.

We now consider two sets of DFAs: the set $\mathfrak{F}$ of minimal DFAs recognizing finite languages, and the set $\mathfrak{G}$ of acyclic and initially connected DFAs with a unique sink. From Lemmas 2 and 3, $\mathfrak{F}$ consists of precisely the automata in $\mathfrak{G}$ that also possess the state uniqueness.

In order to derive our recurrence, we first transform DFAs in $\mathfrak{G}$ into decorated lattice paths that we call *B-paths*. For a given $A \in \mathfrak{G}$, our first step is to construct a spanning subtree of A (excluding the sink) using a depth-first search (*DFS* hereinafter) from the initial state q_0 as shown in Figure 2. This DFS is uniquely defined by taking edges marked by a before edges marked by b. Since A is initially connected, the tree obtained is a spanning tree.

Using the same DFS, we construct a path P starting at the point $(-1, 0)$ and illustrated by a blue line in Figure 3 as follows:

- Whenever the directed blue line around the tree in Figure 3 goes up we add a *vertical step* $V = (0, 1)$ to the path. We say that the state we just quit *corresponds* to this step.
- Whenever the directed blue line crosses an outgoing edge (including the edge leading to the sink), which is not part of the tree, we add a *horizontal step* $H = (1, 0)$.

The order of states corresponding to V-steps is called the *postorder* of states. It is clear that the first step of P is a H-step, and removing it from P gives a Dyck path under the main diagonal. We now decorate P with spots and crosses. Each step V is decorated by a green or white spot, according to whether the corresponding state is accepting or rejecting.

Since A is acyclic, during the DFS, for an edge e pointing from the current state q to an already visited state q', the state q' must not be an ancestor of q in the constructed tree, meaning that q' must either come before q in postorder or be the sink. In the former case, we put a cross in the cell at the intersection between the column of the H-step corresponding to e, and the row of the V-step corresponding to q', while in the latter case we put the cross in the row just below $y = 0$. Clearly the crosses are under P and above $y = -1$. We thus obtain a path B with decorations, and we say that B is the B-path of the automaton A.

To characterize B-paths obtained from DFAs in $\mathfrak{G}$, we propose the following definition. An *automatic B-path* P of size n is defined as a lattice path consisting of up steps and horizontal steps from $(-1, 0)$ to (n, n) with decorations such that

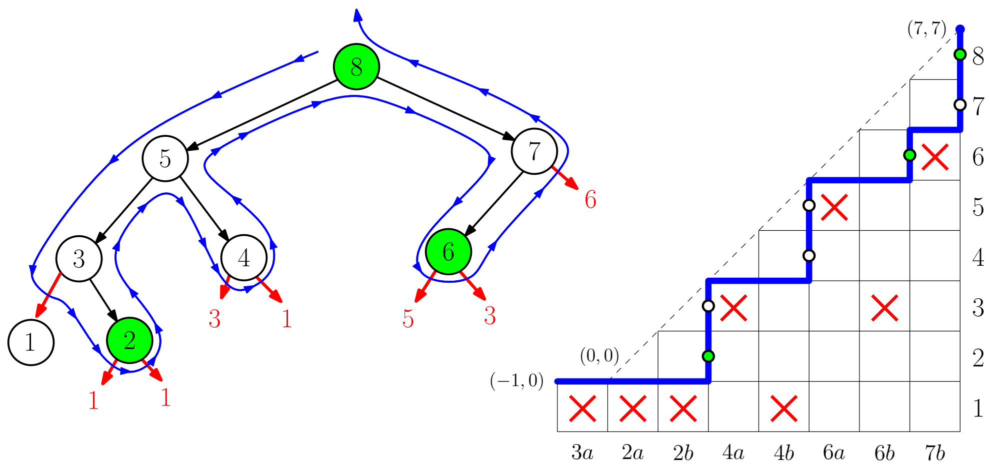


Figure 3 The transformation from an acyclic DFA to a B-path. In the DFA, the states are numbered in order of their corresponding up steps and we have labelled each outgoing edge not in the tree with the number of the state it points to.

- The first step is an H-step, and its removal leaves a Dyck path below the main diagonal;
- Each H-step has a cross in its column, under P and above $y = -1$.
- Every V-step has a white or green spot.

It is not difficult to see that automatic B-paths are in bijection with $\mathfrak{G}$, with the size preserved, since a B-path P obtained from a DFA $A \in \mathfrak{G}$ is clearly automatic, and the construction of B-paths can be easily reversed to obtain a DFA in $\mathfrak{G}$ from an automatic B-path.

Now we examine automatic B-paths corresponding to DFAs in $\mathfrak{F}$. By definition, we only need to take the state uniqueness into account. Given $A \in \mathfrak{G}$, let T be its depth-first search tree and B its corresponding automatic B-path. A state $q \in A$ is called a *cherry* if it is a leaf of T but not the sink. Seen on B, a cherry state corresponds to a sequence HHV of steps. We now propose a seemingly weaker notion of state uniqueness called *cherry-state uniqueness*, which is in fact equivalent in our case.

▶ **Lemma 4.** *Suppose that $A \in \mathfrak{G}$, then A has state uniqueness if and only if it has* cherry-state uniqueness*, i.e., any two states q, q' such that q comes before q' in postorder, and q' is a cherry state, satisfy the conditions in the definition of state uniqueness.*

Proof. State uniqueness clearly implies cherry-state uniqueness. For the other direction, let T be the DFS tree of A. Suppose that we have two states $q \neq q'$ such that $\delta(q, a) = \delta(q', a)$ and $\delta(q, b) = \delta(q', b)$. We suppose that q precedes q' in postorder. It is clear that q' is not an ancestor of q, but q is also not an ancestor of q, or else q would have a transition to itself or to one of its ancestors, which is impossible as A is acyclic. This implies that both $\delta(q, a)$ and $\delta(q, b)$ come before q in postorder, so neither $\delta(q, a)$ nor $\delta(q, b)$ can be a child of q'. Hence, q' is a cherry. Therefore, cherry-state uniqueness implies state uniqueness. ◀

We now try to construct step by step automatic B-paths corresponding to DFAs in $\mathfrak{F}$. We denote by $B_{n,m}$ the set of prefixes ending at (n, m) of such paths. We always start by an H-step from $(-1, 0)$, thus there is exactly one path in $B_{0,0}$. Suppose that we have constructed all automatic B-paths ending at $0 \leq m' \leq m$ and $m' \leq n' \leq n$ except for (n, m), and we now construct paths in $B_{n,m}$. First, from any path in $B_{n-1,m}$, we can construct a path $P \in B_{n,m}$ by adding an H-step at height m with a cross, and there are $(m + 1)$

possibilities for the cross. Second, from any path in $B_{n,m-1}$, we can construct a path P by adding a V-step with a spot that can be green or white. Such a path P ends in a V-step, thus it is different from paths in the first case. However, it may not be in $B_{n,m}$, because it may end in HHV with H-steps at height $m-1$. In such a case it corresponds to a cherry state that violates the cherry-state uniqueness. Such paths violating the condition for $\mathfrak{F}$ are all constructed by adding HHV at the end of paths in $B_{n-2,m-1}$, then adding crosses for the last two H-steps to make the corresponding cherry state "copy" one of the m states precedng it in postorder. Excluding such paths, we obtain all the paths in $B_{n,m}$. In this way, we construct all automatic B-paths corresponding to DFAs in $\mathfrak{F}$. This construction can be translated into the following recurrence.

▶ **Proposition 5.** *Let $b_{n,m}$ be the number of initial segments of automatic B-paths corresponding to DFAs in $\mathfrak{F}$ ending at (n,m). Then*

$$\begin{cases} b_{n,m} &= 2b_{n,m-1} + (m+1)b_{n-1,m} - mb_{n-2,m-1}, & \text{for } n \geq m \geq 1, \\ b_{n,m} &= 0, & \text{for } n < m, \\ b_{n,0} &= 1, & \text{for } n \geq -1. \end{cases}$$

The number $m_{2,n}$ of minimal binary DFAs of size n recognizing a finite language is equal to $b_{n,n}$.

This recurrence relation can be directly used to compute all elements of the sequence $(m_{2,n})_{n\geq 0}$ up to size $n = N$ with $\mathcal{O}(N^2)$ arithmetic operations. The first few numbers of this sequence read

$$(m_{2,n})_{n\geq 0} = (1, 1, 6, 60, 900, 18480, 487560, 15824880, 612504240, 27619664640, \ldots).$$

We have added it as sequence OEIS A331120 in the Online Encyclopedia of Integer Sequences[1]. Previously, the first 7 elements were computed in [5, Section 6].

3 A stretched exponential appears

We now perform an asymptotic analysis of the numbers $m_{2,n}$ using the recurrence derived in the previous section. As a first step we define an auxiliary sequence, which simplifies the subsequent analysis by absorbing the leading exponential behaviour:

$$\tilde{b}_{n,m} = \frac{b_{n,m}}{2^{m-1}}, \qquad \text{for } m \geq 1,$$
$$\tilde{b}_{n,0} = b_{n,0} = 1.$$

This gives

$$\begin{cases} \tilde{b}_{n,m} &= \tilde{b}_{n,m-1} + (m+1)\tilde{b}_{n-1,m} - \frac{m}{2}\tilde{b}_{n-2,m-1}, & \text{for } n \geq m > 1, \\ \tilde{b}_{n,m} &= 0, & \text{for } n < m, \\ \tilde{b}_{n,0} &= 1, & \text{for } n \geq -1. \end{cases}$$

Next, we transform the sequence $(\tilde{b}_{n,m})_{0\leq m\leq n}$ into a sequence $(e_{n,m})_{\substack{0\leq m\leq n \\ n-m \text{ even}}}$ using

$$e_{n,m} = \frac{1}{((n+m)/2)!}\tilde{b}_{(n+m)/2,(n-m)/2},$$

[1] `https://oeis.org`

(note that $e_{n,m}$ is only defined when $n-m$ is even). Then, the terms $e_{n,m}$ are determined by the following recurrence for $n, m \geq 1$

$$\begin{cases} e_{n,m} &= \frac{n-m+2}{n+m} e_{n-1,m-1} + e_{n-1,m+1} - \frac{n-m}{(n+m)(n+m-2)} e_{n-3,m-1}, & \text{for } n \geq m \geq 0, \\ e_{0,0} &= 1, & \\ e_{n,m} &= 0, & \text{for } n < m, \\ e_{n,-1} &= 0, & \text{for } n \geq -1. \end{cases}$$

The number of minimal DFAs of size n is equal to $n!2^{n-1}e_{2n,0}$. Now, for some simple cases of $e_{n,m}$, elementary computations show that $e_{n,n} = \frac{1}{n!}$, $e_{n,n-2} = \frac{2^{n-1}-1}{(n-1)!}$, and $e_{n,n-4} = \frac{3^{n-2}-3 \cdot 2^{n-3}}{(n-2)!}$. Comparing the recurrence above with the one of compacted binary trees given in [6, Section 5] for $e_{n,m}$, we notice only two differences:

1. a slightly different factor $\frac{2(n-m-2)}{(n+m)(n+m-2)}$ of $e_{n-3,m-1}$ and
2. no special cases for $n \geq m > n-3$.

Therefore, we are anticipating the same method to be applicable. The very basic idea is that we will prove lower and upper bounds which differ only in the constant term. This method requires that the recurrence involves only non-negative terms on the right-hand side. As in the case of compacted binary trees, we solve this problem by finding suitable upper and lower bounds given in the subsequent Lemma. We omit its technical proof as it follows exactly the same lines as [6, Lemma 5.1].

▶ **Lemma 6.** *For $n-3 \geq m \geq 2$, the term $e_{n,m}$ is bounded below by*

$$L_e = \frac{n-m+2}{n+m} e_{n-1,m-1} + \frac{n-m-1}{n-m} e_{n-1,m+1} + \frac{n-m-3}{n-m-2} \left(\frac{1}{n-m} e_{n-2,m+2} + \frac{1}{n+m} e_{n-3,m+1} \right)$$

and for $n \geq 5, n > m \geq 0$ bounded above by

$$U_e = \frac{n-m+2}{n+m} e_{n-1,m-1} + \frac{n-m-1}{n-m} e_{n-1,m+1} + \frac{1}{n-m} e_{n-2,m+2} + \frac{1}{n+m} e_{n-3,m+1}.$$

That is, $L_e(n,m) \leq e_{n,m} \leq U_e(n,m)$.

3.1 Lower bound

The following technical Lemma is at the heart of the following inductive proof of the lower bound. It links the recurrence of $e_{n,m}$ (or rather its lower bound L_e) with two explicit sequences $\tilde{s}_n$ and $\tilde{X}_{n,m}$ involving the Airy function, shifted to its right-most root a_1.

▶ **Lemma 7.** *For all $n, m \geq 0$ let*

$$\tilde{X}_{n,m} := \left(1 - \frac{2m^2}{3n} + \frac{3m}{8n}\right) \operatorname{Ai}\left(a_1 + \frac{2^{1/3}(m+1)}{n^{1/3}}\right) \qquad \text{and}$$

$$\tilde{s}_n := 2 + \frac{2^{2/3}a_1}{n^{2/3}} + \frac{29}{12n} - \frac{1}{n^{7/6}}.$$

Then, for any $\varepsilon > 0$, there exists a constant $\tilde{n}_0$ such that

$$\begin{aligned} \tilde{X}_{n,m}\tilde{s}_n\tilde{s}_{n-1}\tilde{s}_{n-2} \leq{}& \frac{n-m+2}{n+m}\tilde{X}_{n-1,m-1}\tilde{s}_{n-1}\tilde{s}_{n-2} + \frac{n-m-1}{n-m}\tilde{X}_{n-1,m+1}\tilde{s}_{n-1}\tilde{s}_{n-2} \\ &+ \frac{n-m-3}{n-m-2}\left(\frac{1}{n-m}\tilde{X}_{n-2,m+2}\tilde{s}_{n-2} + \frac{1}{n+m}\tilde{X}_{n-3,m+1}\right), \end{aligned}$$

for all $n \geq \tilde{n}_0$ and all $0 \leq m < n^{2/3-\varepsilon}$.

Let us show how this Lemma is used before stating its actual proof. First, we define the sequence $X_{n,m} := \max\{\tilde{X}_{n,m}, 0\}$ (note that the factor $1 - \frac{2m^2}{3n} + \frac{3m}{8n}$ is negative for large m). Then, using Lemma 7 we have

$$\begin{aligned} X_{n,m}\tilde{s}_n\tilde{s}_{n-1}\tilde{s}_{n-2} \leq& \frac{n-m+2}{n+m}X_{n-1,m-1}\tilde{s}_{n-1}\tilde{s}_{n-2} + \frac{n-m-1}{n-m}X_{n-1,m+1}\tilde{s}_{n-1}\tilde{s}_{n-2} \\ &+ \frac{n-m-3}{n-m-2}\left(\frac{1}{n-m}X_{n-2,m+2}\tilde{s}_{n-2} + \frac{1}{n+m}X_{n-3,m+1}\right), \end{aligned}$$

for n large enough and all $m \leq n$. Finally, we define the sequence $\tilde{h}_n$ such that $\tilde{h}_n = \tilde{s}_n\tilde{h}_{n-1}$ for $n > 0$ and set $\tilde{h}_0 = \tilde{s}_0$. Then we deduce by induction that $e_{n,m} \geq b_0\tilde{h}_n X_{n,m}$ for some constant $b_0 > 0$, all sufficiently large n, and all $m \in [0, n]$:

$$\begin{aligned} b_0 X_{n,m}\tilde{h}_n \leq& \frac{n-m+2}{n+m}e_{n-1,m-1} + \frac{n-m-1}{n-m}e_{n-1,m+1} + \frac{n-m-3}{n-m-2}\left(\frac{e_{n-2,m+2}}{n-m} + \frac{e_{n-3,m+1}}{n+m}\right) \\ \leq& \, e_{n,m}, \end{aligned}$$

where the first inequality follows by induction and the second one by Lemma 6 for $m \leq n-3$. For $m > n-3$ and n large enough the inequality holds trivially as $X_{n,m} = 0$. Therefore,

$$\begin{aligned} m_{2,n} &= n!2^{n-1}e_{2n,0} \\ &\geq b_0 n!2^{n-1}\tilde{h}_{2n}X_{2n,0} \\ &\geq b_0 n!2^{n-1}\prod_{i=1}^{2n}\left(2 + \frac{2^{2/3}a_1}{i^{2/3}} + \frac{29}{12i} - \frac{1}{i^{7/6}}\right)\mathrm{Ai}\left(a_1 + \frac{1}{n^{1/3}}\right) \\ &\geq \gamma_{\mathrm{L}} n!8^n e^{3a_1 n^{1/3}} n^{7/8}, \end{aligned} \tag{2}$$

for some constant $\gamma_{\mathrm{L}} > 0$.

▶ Remark 8. Let us compare the result of Lemma 7 to the respective results for compacted and relaxed binary trees to which this method was applied first. Recall the lower and upper bounds (1) which are tight up to the constant and the polynomial term. Indeed, the corresponding results [6, Lemmas 4.2 and 5.2] possess a very similar structure: First, in $\tilde{X}_{n,m}$ the only difference is in the factor $\frac{3m}{8n}$ which is $\frac{m}{2n}$ for relaxed trees and $\frac{m}{4n}$ for compacted trees. The purpose of this term is of technical nature as it simplifies the Newton polygon method, yet it has no influence on the final asymptotics; compare Figure 5. Second, in $\tilde{s}_n$ the only difference is in the term $\frac{29}{12n}$ which is $\frac{8}{3n}$ for relaxed trees and $\frac{13}{6n}$ for compacted trees. Now this term influences the polynomial factor in the asymptotics (compare with [6, Section 3.3]). More generally, whenever the third term in the expansion of $\tilde{s}_n$ has the form $\frac{\alpha}{n}$, we get in the enumeration a polynomial factor with exponent $\frac{\alpha}{2} - \frac{1}{3}$. Finally, the similarity in all other terms of the expansion for $\tilde{s}_n$ and $\tilde{X}_{n,m}$ is responsible for the fact that $m_{2,n}$ and the families of trees enumerated in [6] have the same exponential growth, as well as the same stretched-exponential behaviour.

Proof (Lemma 7). The proof follows nearly verbatim [6, Lemma 4.2], so we will only introduce the main idea, omitting the technical details. Note that all (often tedious) computations are available in the accompanying Maple worksheet [12].

We start by defining the following sequence

$$\begin{aligned} P_{n,m} :=& -Z_{n,m}s_n s_{n-1}s_{n-2} \\ &+ \frac{n-m+2}{n+m}Z_{n-1,m-1}s_{n-1}s_{n-2} + \frac{n-m-1}{n-m}Z_{n-1,m+1}s_{n-1}s_{n-2} \\ &+ \frac{n-m-3}{n-m-2}\left(\frac{1}{n-m}Z_{n-2,m+2}s_{n-2} + \frac{1}{n+m}Z_{n-3,m+1}\right), \end{aligned}$$

where

$$s_n := \sigma_0 + \frac{\sigma_1}{n^{1/3}} + \frac{\sigma_2}{n^{2/3}} + \frac{\sigma_3}{n} + \frac{\sigma_4}{n^{7/6}},$$
$$Z_{n,m} := \left(1 + \frac{\tau_2 m^2 + \tau_1 m}{n}\right) \mathrm{Ai}\left(a_1 + \frac{2^{1/3}(m+1)}{n^{1/3}}\right),$$

with $\sigma_i, \tau_j \in \mathbb{R}$. Then the inequality is equivalent to $P_{n,m} \geq 0$ with $\sigma_0 = 2$, $\sigma_1 = 0$, $\sigma_2 = 2^{2/3}a_1$, $\sigma_3 = 29/12$, and $\sigma_4 = -1$ as well as $\tau_1 = 3/8$ and $\tau_2 = -2/3$. Next, we expand $\mathrm{Ai}(z)$ in a neighborhood of

$$\alpha = a_1 + \frac{2^{1/3}m}{n^{1/3}}, \tag{3}$$

and we get

$$P_{n,m} = p_{n,m}\mathrm{Ai}(\alpha) + p'_{n,m}\mathrm{Ai}'(\alpha),$$

where $p_{n,m}$ and $p'_{n,m}$ are functions of m and n^{-1} and may be expanded as power series in $n^{-1/6}$ with coefficients polynomial in m. We will see that, as long as $n > 1$ and $n > m$, this series converges absolutely because the Airy function is entire and so all the functions for which we need to perform a bivariate expansion (in n and m) are indeed are analytic in the region defined by $|n| > 1$ and $|m| < |n|^{2/3-\varepsilon}$.

Now we proceed with the technical analysis, which is only performed on a superficial level here. The first step is to show that $[m^i n^j]P_{n,m} = 0$ for $i + j > 1$, $i, j \in \mathbb{Q}$. Then, as a second step, we strengthen this result by choosing suitable values σ_i for $0 \leq i \leq 4$ in the definition of s_n in order to eliminate more terms. The results are summarized in Figure 4 where the initial non-zero coefficients are shown. A diamond at (i, j) is drawn if and only if the coefficient $[m^i n^j]P_{n,m}$ is non-zero for generic values of σ and τ. It is an empty diamond if the given choice of σ_i and τ_j makes it vanish, whereas it is a solid diamond if it remains non-zero. The convex hull is formed by the following three lines

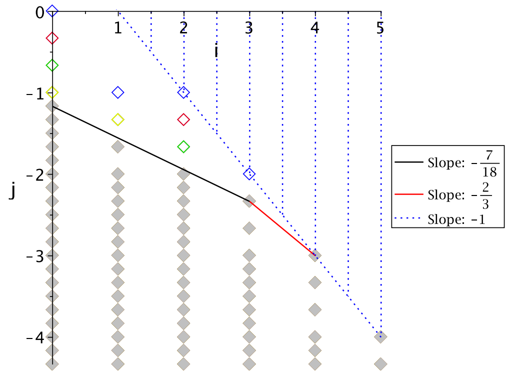
$$L_1 : j = -\frac{7}{6} - \frac{7i}{18}, \qquad L_2 : j = -\frac{1}{3} - \frac{2i}{3}, \qquad L_3 : j = 1 - i.$$

From now on, we distinguish between the contributions arising from $p_{n,m}$ and $p'_{n,m}$. The non-zero coefficients are shown in Figure 5. For technical reasons we choose at this point $\tau_1 = 8/3$ and thereby reduce the slope of the convex hull of the non-zero coefficients of $p'_{n,m}$. The expansions for n tending to infinity start as follows, where the elements on the convex hull are written in color:

$$\begin{aligned} P_{n,m} = \mathrm{Ai}(\alpha) &\left(-\frac{4\sigma_4}{n^{7/6}} - \frac{2^{11/3}a_1 m}{3n^{5/3}} - \frac{164m^2}{9n^2} - \frac{2^{14/3}a_1 m^3}{3n^{8/3}} - \frac{136m^4}{9n^3} - \frac{248m^5}{135n^4} + \dots\right) + \\ \mathrm{Ai}'(\alpha) &\left(\frac{2^{1/3}(8\tau_1 - 3)}{n^{4/3}} + \frac{2^{7/3}}{n^{3/2}} - \frac{32a_1 m}{9n^2} + \frac{2^{4/3}m^2(48\tau_1 - 65)}{9n^{7/3}} - \frac{2^{19/3}m^3}{9n^{7/3}}\right. \\ &\left. -5\frac{2^{10/3}m^4}{9n^{10/3}} - 89\frac{2^{10/3}m^5}{135n^{13/3}} + \dots\right). \end{aligned}$$

We now choose $\sigma_4 = -1$ which leads to a positive term $\mathrm{Ai}(\alpha)n^{-7/6}$. Next, for fixed (large) n we prove that for all m the dominant contributions in $P_{n,m}$ are positive. Motivated by Figures 4 and 5, we consider three different regimes: $m \leq Cn^{1/3}$, $Cn^{1/3} < m \leq n^{7/18}$, and $n^{7/18} < m < n^{2/3-\epsilon}$ for a suitable constant $C > 0$. We end the proof by showing that there exists an $N > 0$ such that all terms are positive for $n > N$ and all $m < n^{2/3}$. ◀

In the next section we will show an upper bound with the same asymptotic form, but with a different constant γ_U.



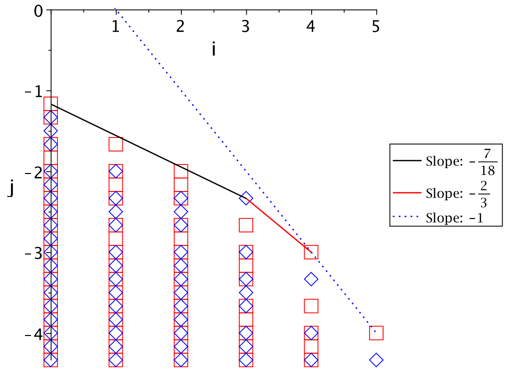


Figure 4 (Left) Non-zero coefficients of $P_{n,m} = \sum a_{i,j} m^i n^j$ shown by diamonds for $s_n := \sigma_0 + \frac{\sigma_1}{n^{1/3}} + \frac{\sigma_2}{n^{2/3}} + \frac{\sigma_3}{n} + \frac{\sigma_4}{n^{7/6}}$ and $Z_{n,m} := \left(1 + \frac{\tau_2 m^2 + \tau_1 m}{n}\right) \operatorname{Ai}\left(a_1 + \frac{2^{1/3}(m+1)}{n^{1/3}}\right)$. There are no terms in the blue dashed area. The blue terms vanish for $\sigma_0 = 2$, the red terms vanish for $\sigma_1 = 0$, the green terms vanish for $\sigma_2 = 2^{2/3} a_1$, and the yellow terms vanish for $\sigma_3 = 29/12$ and $\tau_2 = -2/3$. The black and red lines represent the two parts L_1 and L_2, respectively, of the convex hull. (Right) The solid gray diamonds are decomposed into the coefficients $p_{n,m}$ of $\operatorname{Ai}(\alpha)$ (red boxes) and $p'_{n,m}$ of $\operatorname{Ai}'(\alpha)$ (blue diamonds).

3.2 Upper bound

The following lemma links as in the case of the lower bound $e_{n,m}$ (and its upper bound U_e) with two explicit sequences $\hat{s}_n$ and $\hat{X}_{n,m}$ involving again the Airy function.

▶ **Lemma 9.** *Choose $\eta > 2/9$ fixed and for all $n, m \geq 0$ let*

$$\hat{X}_{n,m} := \left(1 - \frac{2m^2}{3n} + \frac{3m}{8n} + \eta \frac{m^4}{n^2}\right) \operatorname{Ai}\left(a_1 + \frac{2^{1/3}(m+1)}{n^{1/3}}\right) \qquad \text{and}$$

$$\hat{s}_n := 2 + \frac{2^{2/3} a_1}{n^{2/3}} + \frac{29}{12n} + \frac{1}{n^{7/6}}.$$

Then, for any $\varepsilon > 0$, there exists a constant $\hat{n}_0$ such that

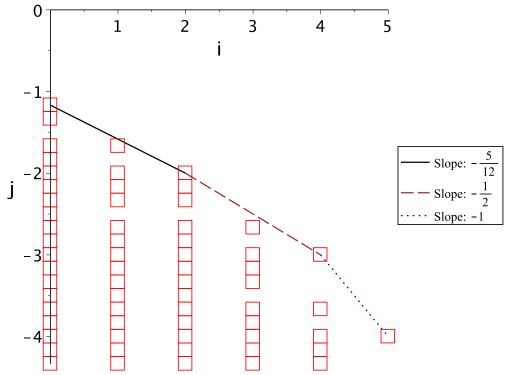
$$\begin{aligned} \hat{X}_{n,m}\hat{s}_n\hat{s}_{n-1}\hat{s}_{n-2} \geq \frac{n-m+2}{n+m}\hat{X}_{n-1,m-1}\tilde{s}_{n-1}\tilde{s}_{n-2} + \frac{n-m-1}{n-m}\hat{X}_{n-1,m+1}\tilde{s}_{n-1}\tilde{s}_{n-2} \\ + \frac{1}{n-m}\hat{X}_{n-2,m+2}\tilde{s}_{n-2} + \frac{1}{n+m}\hat{X}_{n-3,m+1}, \end{aligned} \tag{4}$$

for all $n \geq \hat{n}_0$ and all $0 \leq m < n^{1-\varepsilon}$.

Proof (Sketch). The proof follows the same lines as that of Lemma 7, so we will only elucidate the required modifications. As a first step we define the following sequence

$$\begin{aligned} Q_{n,m} := \hat{X}_{n,m}\hat{s}_n\hat{s}_{n-1}\hat{s}_{n-2} - \frac{n-m+2}{n+m}\hat{X}_{n-1,m-1}\tilde{s}_{n-1}\tilde{s}_{n-2} - \frac{n-m-1}{n-m}\hat{X}_{n-1,m+1}\tilde{s}_{n-1}\tilde{s}_{n-2} \\ - \frac{1}{n-m}\hat{X}_{n-2,m+2}\tilde{s}_{n-2} - \frac{1}{n+m}\hat{X}_{n-3,m+1}. \end{aligned}$$

Then the inequality is equivalent to $Q_{n,m} \geq 0$. Again, we expand $\operatorname{Ai}(z)$ in a neighborhood of $\alpha = a_1 + \frac{2^{1/3} m}{n^{1/3}}$, and we get the following expansion (see the accompanying Maple worksheet [12] for full details). As before, the elements on the convex hull are written in color.



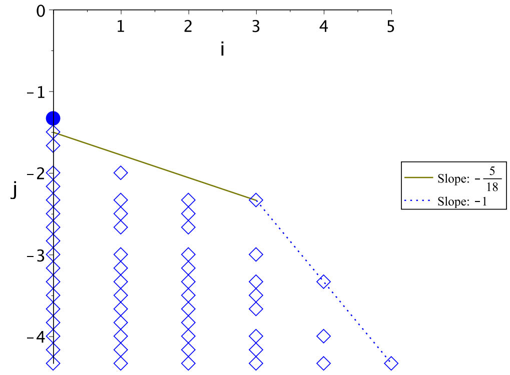


Figure 5 Non-zero coefficients $p_{n,m} = \sum \tilde{a}_{i,j} m^i n^j$ (red) and $p'_{n,m} = \sum \tilde{a}'_{i,j} m^i n^j$ (blue) of the expansion (3) for $P_{n,m}$. The coefficient of $n^{-4/3}$ in the right picture depicted as a solid blue circle disappears for $\tau_1 = 3/8$.

$$\begin{aligned}Q_{n,m} = \operatorname{Ai}(\alpha)\Bigg(&\frac{4}{n^{7/6}} + \frac{2^{11/3}a_1 m}{3n^{5/3}} + \frac{4m^2(41-108\eta)}{9n^2} + \frac{2^{14/3}a_1 m^3(1-6\eta)}{3n^{8/3}}\\ &+\frac{8m^4(17-132\eta)}{9n^3} - \frac{2^{11/3}a_1 m^5\eta}{n^{11/3}} - \frac{68m^6\eta}{3n^4} - \frac{124m^7\eta}{45n^5} + \dots\Bigg) +\\ \operatorname{Ai}'(\alpha)\Bigg(&\frac{2^{7/3}}{n^{3/2}} + \frac{32a_1 m}{9n^2} + \frac{2^{4/3}m^2(47-216\eta)}{9n^{7/3}} + \frac{2^{16/3}m^3(2-9\eta)}{9n^{7/3}}\\ &+\frac{2^{1/3}m^4(40-549\eta)}{9n^{10/3}} - \frac{2^{16/3}m^5\eta}{3n^{10/3}} - \frac{5m^6 2^{7/3}\eta}{3n^{13/3}} - \frac{89m^7 2^{7/3}\eta}{45n^{16/3}} + \dots\Bigg).\end{aligned}$$

Then we can finish in the same way as in the proof of Lemma 7. For the full details we refer to the proofs of [6, Lemma 4.4 and 5.3] which explains how to deal with the new cases required in the treatment of the upper bound (that happen to be analogous for the sequence at hand here, and the ones in that paper). Note that even the final convex hull in the Newton polygons is the same. ◀

The idea is now similar to the lower bound, yet a bit more intricate: We want to find an auxiliary sequence $(\tilde{e}_{n,m})_{n,m\geq 0}$ satisfying $e_{n,m} \leq C\tilde{e}_{n,m}$ for some constant $C > 0$, all n large, and all $m \leq n$ such that

$$\tilde{e}_{n,m} \leq \kappa_1 \hat{h}_n \hat{X}_{n,m}, \tag{5}$$

where the sequence $(\hat{h}_n)_{n\geq 1}$ is defined by $\hat{h}_n = \hat{s}_n \hat{h}_{n-1}$. As shown in (2), this implies that there is a constant $\gamma_{\mathrm{U}} > 0$ such that

$$\tilde{e}_{2n,0} \leq \gamma_{\mathrm{U}} 4^n e^{3a_1 n^{1/3}} n^{7/8}.$$

Now, in order to find such a sequence we use Lemma 6 and state the following definition for $(\tilde{e}_{n,m})_{n,m\geq 0}$:

$$\begin{cases} \tilde{e}_{n,m} = \frac{n-m+2}{n+m}\tilde{e}_{n-1,m-1} + \frac{n-m-1}{n-m}\tilde{e}_{n-1,m+1} \\ \qquad + \frac{1}{n-m}\tilde{e}_{n-2,m+2} + \frac{1}{n+m}\tilde{e}_{n-3,m+1}, & \text{for } n \geq 5, n^{3/4} > m \geq 0, \\ \tilde{e}_{n,m} = e_{n,m}, & \text{for } n < 5, n \geq m \geq 0, \\ \tilde{e}_{n,m} = 0, & \text{otherwise.} \end{cases} \tag{6}$$

There are several ideas in the choice of the sequence (6) which we want to explain now. Firstly, in order to prove (5), the sequence has to be zero for large values of m. We achieve this by cutting off the values for $m > n^{3/4}$. Secondly, it has to have positive coefficients, because then we can prove (5) by induction as it was done in the lower bound. Thirdly, it has to be an upper bound of $e_{n,m}$, i.e., $e_{n,m} \leq C\hat{e}_{n,m}$ for all n, m. Due to the cut off for $m > n^{3/4}$ this is, of course, impossible, so we introduce a second auxiliary sequence $(\hat{e}_{n,m})_{n,m\geq 0}$ with the same rules as (6) yet with no cut off, i.e., the recurrence holds for $n \geq 5$ and $n > m \geq 0$. Then, by Lemma 6 we have $e_{n,m} \leq \hat{e}_{n,m}$ for all n, m.

Hence, it remains to prove that there is a choice of N and a constant $C > 0$ such that

$$\hat{e}_{2n,0} \leq C\tilde{e}_{2n,0}$$

for all $n > N$. As a first step, we define a class $\mathcal{C}$ of weighted paths with the step set $\mathcal{S} := \{(1,1), (1,-1), (2,-2), (3,-1)\}$ and weights corresponding to the recurrence defining $\hat{e}_{n,m}$. Then $\hat{e}_{n,m}$ can be interpreted as the weighted enumeration of paths $p_0p_1 \dots p_k \in \mathcal{C}$ ($p_i \in \mathbb{Z}^2$) from p_0 to $p_k = (n,m)$ such that $p_{i+1} - p_i \in \mathcal{S}$ for $0 \leq i \leq k-1$, with the additional initial condition that $p_0 = (u_0, v_0)$ and $p_1 = (u_1, v_1)$ satisfy $v_0 \leq u_0 < 5 \leq u_1$. In other words, the first jump $p_1 - p_0$ has to exit $\mathcal{I} := \{(i,j) : i < 5\}$. The weight given to each path in this enumeration is e_{u_0,v_0}

▶ **Lemma 10.** *Let $q_{\ell,m,2n}$ denote the weighted number of paths $p \in \mathcal{C}$ from (ℓ, m) to $(2n, 0)$. Then the numbers $q_{\ell,m,2n}$ satisfy the inequality*

$$\frac{q_{\ell,j,2n}}{j+1} \geq \frac{q_{\ell,k,2n}}{k+1},$$

for integers $0 \leq j < k \leq \ell \leq 2n$ satisfying $2|k-j$ and $n \geq 10$.

Proof (Sketch). Reversing the steps in (6) we see that q satisfies the following recurrence for $\ell < 2n$:

$$\begin{cases} q_{\ell,m,2n} &= 0, & \text{for} \quad m < 0, \\ q_{\ell,m,2n} &= \frac{\ell-m+1}{\ell-m+2} q_{\ell+1,m-1,2n} + \frac{\ell-m+2}{\ell+m+2} q_{\ell+1,m+1,2n} & \\ &\quad + \frac{1}{\ell-m+4} q_{\ell+2,m-2,2n} + \frac{1}{\ell+m+2} q_{\ell+3,m-1,2n} & \text{for} \quad m \geq 0. \end{cases}$$

Then we follow nearly verbatim the lines of the proof of [6, Lemma 5.4]. For more details we refer to the accompanying Maple worksheet [12]. ◀

The last ingredient we will need is that

$$\hat{e}_{2x,2y} \leq d_{2x,2y} \leq \binom{2x}{x+y},$$

where the sequence $d_{x,y}$ corresponds to the weighted number of Dyck meanders of length x ending at y; see [6, Proposition 3.2]. The first inequality is proved by induction using the recurrence relations of $\hat{e}_{x,y}$ and $d_{x,y}$. The second inequality is proved in [6], yet simply a consequence of the fact that $\binom{2x}{x+y}$ is the (unweighted) number of Dyck meanders from $(0,0)$ to $(2x, 2y)$, while the weights of weighted Dyck meanders are always smaller than 1.

Finally, among the $\hat{e}_{2n,0}$ weighted paths ending at $(2n, 0)$, the proportion of those passing through some point $(2x, 2y)$ is

$$\frac{\hat{e}_{2x,2y} q_{2x,2y,2n}}{\hat{e}_{2n,0}} \leq \frac{\hat{e}_{2x,2y} q_{2x,2y,2n}}{\hat{e}_{2x,0} q_{2x,0,2n}} \leq (2y+1) \frac{\hat{e}_{2x,2y}}{\hat{e}_{2x,0}} \leq \frac{2y+1}{\gamma_{\mathrm{L}} 4^x e^{3a_1 x^{1/3}} x^{3/4}} \binom{2x}{x+y}.$$

In the last inequality we used Lemma 10 as well as $e_{n,m} \leq \hat{e}_{n,m}$ and the lower bound (2) for $\hat{e}_{2x,0}$. Hence, we can use the same ideas as used in [6, Lemma 4.6] to show that there is some choice for N such that $\hat{e}_{2n,0} \leq 2\tilde{e}_{2n,0}$ for all n.

This proves the missing link and ends the proof of Theorem 1.

To conclude, we observe that all arguments in Section 2 can be extended to any finite alphabet of any size at least 2. Our analysis may also be extended to this more general case, but this remains a work in progress.

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The First Bijective Proof of the Alternating Sign Matrix Theorem Theorem

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Abstract

Alternating sign matrices are known to be equinumerous with descending plane partitions, totally symmetric self-complementary plane partitions and alternating sign triangles, but a bijective proof for any of these equivalences has been elusive for almost 40 years. In this extended abstract, we provide a sketch of the first bijective proof of the enumeration formula for alternating sign matrices, and of the fact that alternating sign matrices are equinumerous with descending plane partitions. The bijections are based on the operator formula for the number of monotone triangles due to the first author. The starting point for these constructions were known "computational" proofs, but the combinatorial point of view led to several drastic modifications and simplifications. We also provide computer code where all of our constructions have been implemented.

2012 ACM Subject Classification Mathematics of computing → Combinatoric problems; Mathematics of computing → Combinatorial algorithms; Mathematics of computing → Enumeration

Keywords and phrases enumeration, bijective proof, alternating sign matrix, plane partition

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.12

Related Version A full version of the paper is available at [14, 15], https://arxiv.org/abs/1910.04198, https://arxiv.org/abs/1912.01354.

Funding *Ilse Fischer*: Austrian Science Foundation FWF, SFB grant F50.
Matjaž Konvalinka: Slovenian Research Agency (research core funding No. P1-0294).

1 Introduction

An *alternating sign matrix* (ASM) is a square matrix with entries in $\{0, 1, -1\}$ such that in each row and each column the non-zero entries alternate and sum up to 1. Robbins and Rumsey introduced alternating sign matrices in the 1980s [22] when studying their λ-*determinant* (a generalization of the classical determinant) and showing that the λ-determinant can be expressed as a sum over all alternating sign matrices of fixed size. The classical determinant is obtained from this by setting $\lambda = -1$, in which case the sum reduces so that it extends only over all ASMs *without* -1's, i.e., permutation matrices, and the well-known formula of Leibniz is recovered. Numerical experiments led Robbins and Rumsey to conjecture that the number of $n \times n$ alternating sign matrices is given by the surprisingly simple product formula

$$\prod_{i=0}^{n-1} \frac{(3i+1)!}{(n+i)!}. \tag{1}$$

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 12; pp. 12:1–12:12
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

Back then the surprise was even bigger when they learned from Stanley (see [9, 8]) that this product formula had recently also appeared in Andrews' paper [1] on his proof of the weak Macdonald conjecture, which in turn provides a formula for the number of *cyclically symmetric plane partitions*. As a byproduct, Andrews had introduced *descending plane partitions* and had proved that the number of descending plane partitions (DPPs) with parts at most n is also equal to (1). A descending plane partition is a filling of a shifted Ferrers diagram with positive integers that decrease weakly along rows and strictly along columns such that the first part in each row is greater than the length of its row and less than or equal to the length of the previous row.

Since then the problem of finding an explicit bijection between alternating sign matrices and descending plane partitions has attracted considerable attention from combinatorialists, and to many of them it is a miracle that such a bijection has not been found so far. All the more so because Mills, Robbins and Rumsey also introduced several "statistics" on alternating sign matrices and on descending plane partitions for which they had strong numerical evidence that the joint distributions coincide as well, see [20].

There were a few further surprises yet to come. Robbins introduced a new operation on plane partitions, *complementation*, and had strong numerical evidence that totally symmetric self-complementary plane partitions (TSSCPPs) in a $2n \times 2n \times 2n$-box are also counted by (1). Again this was further supported by statistics that have the same joint distribution as well as certain refinements, see [21, 17, 18, 7]. We still lack an explicit bijection between TSSCPPs and ASMs, as well as between TSSCPPs and DPPs.

In his collection of bijective proof problems (which is available from his webpage) Stanley says the following about the problem of finding all these bijections: "*This is one of the most intriguing open problems in the area of bijective proofs.*" In Krattenthaler's survey on plane partitions [18] he expresses his opinion by saying: "*The greatest, still unsolved, mystery concerns the question of what plane partitions have to do with alternating sign matrices.*"

Many of the above mentioned conjectures have since been proved by non-bijective means. Zeilberger [24] was the first who proved that $n \times n$ ASMs are counted by (1). Kuperberg gave another shorter proof [19] based on the remarkable observation that the *six-vertex model* (which had been introduced by physicists several decades earlier) with domain wall boundary conditions is equivalent to ASMs, and he used the techniques that had been developed by physicists to study this model. Andrews enumerated TSSCPPs in [2]. The equivalence of certain statistics for ASMs and of certain statistics for DPPs has been proved in [5], while for ASMs and TSSCPPs see [25, 16], and note in particular that already in Zeilberger's first ASM paper [24] he could deal with an important refinement. Further work including the study of *symmetry classes* has been accomplished; for a more detailed description of this we defer to [6]. Then, in very recent work, alternating sign triangles (ASTs) were introduced in [3], which establishes a fourth class of objects that are equinumerous with ASMs, and also in this case nobody has so far been able to construct a bijection.

The first author gave her "own" proof of the ASM theorem in [11, 12, 13] and expressed some speculations in the direction of converting these proofs into bijections in the final section of the last paper. Part of the objective, namely bijective proofs of the enumeration formula for the number of ASMs and of the fact that ASMs and DPPs are equinumerous, has now been achieved in [14, 15], the first two papers in a planned series. This extended abstract presents the major steps in these constructions.

After having figured out how to actually convert computations and also having shaped certain useful fundamental concepts related to *signed sets* (see Section 2), the translation of several steps became quite straightforward; some steps were quite challenging. Then a certain type of (exciting) dynamics evolved, where the combinatorial point of view led to simplifications and other (in some cases drastic) modifications, and after this process the original "computational" proof is in fact rather difficult to recognize.

The bijection that underlies the bijective proof of the enumeration formula of ASMs as well as the one of the refined enumeration formula involves the following sets:

- Let ASM_n denote the set of ASMs of size $n \times n$, and, for $1 \le i \le n$, let $\mathrm{ASM}_{n,i}$ denote the subset of ASM_n of matrices that have the unique 1 in the first row in column i. There is an obvious bijection $\mathrm{ASM}_{n,1} \to \mathrm{ASM}_{n-1}$ which consists of deleting the first row and first column.
- Let B_n denote the set of $(2n-1)$-subsets of $[3n-2] = \{1, 2, \ldots, 3n-2\}$ and, for $1 \le i \le n$, let $\mathrm{B}_{n,i}$ denote the subset of B_n of those subsets whose median is $n+i-1$. Clearly, $|\mathrm{B}_n| = \binom{3n-2}{2n-1}$ and $|\mathrm{B}_{n,i}| = \binom{n+i-2}{n-1}\binom{2n-i-1}{n-1}$.
- Let DPP_n denote the set of descending plane partitions with parts no greater than n; let $\mathrm{DPP}_{n,i}$ the subset of descending plane partitions with $i-1$ occurrences of n. We clearly have $\mathrm{DPP}_{n,1} = \mathrm{DPP}_{n-1}$.

To emphasize that we are not merely interested in the fact that two signed sets have the same size, but want to use the constructed signed bijection later on, we will be using a convention that is slightly unorthodox in our field. Instead of listing our results as lemmas and theorems with their corresponding proofs, we will be using the Problem–Construction terminology. See for instance [23] and [4]. Our main results are the constructions solving the following two problems.

▶ **Problem 1** ([15, Problem 1]). *Given $n \in \mathbb{N}$, $1 \le i \le n$, construct a bijection*

$$\mathrm{DPP}_{n-1} \times \mathrm{B}_{n,1} \times \mathrm{ASM}_{n,i} \longrightarrow \mathrm{DPP}_{n-1} \times \mathrm{ASM}_{n,1} \times \mathrm{B}_{n,i}\,.$$

Assume that we have constructed such bijections. Then we also have a bijection

$$\begin{aligned}&\mathrm{DPP}_{n-1} \times \mathrm{B}_{n,1} \times \mathrm{ASM}_n = \bigcup_i (\mathrm{DPP}_{n-1} \times \mathrm{B}_{n,1} \times \mathrm{ASM}_{n,i})\\ &\longrightarrow \bigcup_i (\mathrm{DPP}_{n-1} \times \mathrm{ASM}_{n,1} \times \mathrm{B}_{n,i}) = \mathrm{DPP}_{n-1} \times \mathrm{ASM}_{n,1} \times \mathrm{B}_n \longrightarrow \mathrm{DPP}_{n-1} \times \mathrm{ASM}_{n-1} \times \mathrm{B}_n\end{aligned}$$

for every n. But by induction, that gives a bijection

$$\mathrm{DPP}_0 \times \cdots \times \mathrm{DPP}_{n-1} \times \mathrm{B}_{1,1} \times \cdots \times \mathrm{B}_{n,1} \times \mathrm{ASM}_n \longrightarrow \mathrm{DPP}_0 \times \cdots \times \mathrm{DPP}_{n-1} \times \mathrm{B}_1 \times \cdots \times \mathrm{B}_n,$$

which, since DPP_i is non-empty (as it contains the empty DPP), proves the ASM theorem

$$|\mathrm{ASM}_n| = \frac{\prod_{i=1}^n |\mathrm{B}_i|}{\prod_{i=1}^n |\mathrm{B}_{i,1}|} = \frac{\prod_{i=1}^n \binom{3i-2}{2i-1}}{\prod_{i=1}^n \binom{2i-2}{i-1}} = \prod_{i=0}^{n-1} \frac{(3i+1)!}{(n+i)!}$$

and also the refined ASM theorem

$$|\mathrm{ASM}_{n,i}| = \frac{|\mathrm{ASM}_{n-1}| \cdot |\mathrm{B}_{n,i}|}{|\mathrm{B}_{n,1}|} = \frac{\binom{n+i-2}{n-1}\binom{2n-i-1}{n-1}}{\binom{3n-2}{2n-1}} \prod_{i=0}^{n-1} \frac{(3i+1)!}{(n+i)!}.$$

Next we provide the bijection from Problem 1 for the case $n = 3$ and $i = 2$; in fact, our bijection depends on an integer parameter x and we choose $x = 0$.

$$
\begin{array}{ccccccccc}
\left(\varnothing, 12345, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 23457\right) & \left(\varnothing, 12345, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 23456\right) & \left(\varnothing, 12345, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 23456\right) \\
\left(\varnothing, 12346, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 13457\right) & \left(\varnothing, 12346, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 13456\right) & \left(\varnothing, 12346, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 13456\right) \\
\left(\varnothing, 12347, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 12457\right) & \left(\varnothing, 12347, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 12456\right) & \left(\varnothing, 12347, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 12456\right) \\
\left(\varnothing, 12356, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 13456\right) & \left(\varnothing, 12356, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 12456\right) & \left(\varnothing, 12356, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 12456\right) \\
\left(\varnothing, 12357, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 13457\right) & \left(\varnothing, 12357, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 12457\right) & \left(\varnothing, 12357, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 12457\right) \\
\left(\varnothing, 12367, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 13467\right) & \left(\varnothing, 12367, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 12467\right) & \left(\varnothing, 12367, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 12467\right) \\
\left(2, 12345, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 23467\right) & \left(2, 12345, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 23467\right) & \left(2, 12345, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 23457\right) \\
\left(2, 12346, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 13467\right) & \left(2, 12346, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 13467\right) & \left(2, 12346, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 13457\right) \\
\left(2, 12347, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 12467\right) & \left(2, 12347, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 12467\right) & \left(2, 12347, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(\varnothing, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 12457\right) \\
\left(2, 12356, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 23456\right) & \left(2, 12356, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 23456\right) & \left(2, 12356, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 13456\right) \\
\left(2, 12357, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 23457\right) & \left(2, 12357, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 23457\right) & \left(2, 12357, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 13457\right) \\
\left(2, 12367, \begin{smallmatrix}0&1&0\\1&0&0\\0&0&1\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&1&0\\0&0&1\end{smallmatrix}, 23467\right) & \left(2, 12367, \begin{smallmatrix}0&1&0\\1&-1&1\\0&1&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 23467\right) & \left(2, 12367, \begin{smallmatrix}0&1&0\\0&0&1\\1&0&0\end{smallmatrix}\right) & \leftrightarrow & \left(2, \begin{smallmatrix}1&0&0\\0&0&1\\0&1&0\end{smallmatrix}, 13467\right)
\end{array}
$$

The second bijection relates ASMs to DPPs.

▶ **Problem 2** ([15, Problem 2]). *Given $n \in \mathbb{N}$, $1 \le j \le n$, construct a bijection*

$$\mathrm{DPP}_{n-1} \times \mathrm{ASM}_{n,j} \longrightarrow \mathrm{ASM}_{n-1} \times \mathrm{DPP}_{n,j}\,.$$

Once this is proven it follows that $|\mathrm{DPP}_{n-1}| \cdot |\mathrm{ASM}_{n,j}| = |\mathrm{ASM}_{n-1}| \cdot |\mathrm{DPP}_{n,j}|$. By induction, we can assume $|\mathrm{DPP}_{n-1}| = |\mathrm{ASM}_{n-1}|$ and so $|\mathrm{ASM}_{n,j}| = |\mathrm{DPP}_{n,j}|$. Summing this over all j implies $|\mathrm{DPP}_n| = |\mathrm{ASM}_n|$.

For several obvious reasons, we found it essential to check all our constructions with computer code[1]; to name one it can possibly be used to identify new equivalent statistics. Another is that it might be possible to find some patterns in the bijection and to simplify the description. Finally, let us emphasize that our approach does give the first bijection of a celebrated result, it fails to explain the simplicity of the product formula for ASMs.

2 Signed sets and sijections

It seems that signs and cancellations in the proof are unavoidable. In this section, we briefly introduce the concepts of *signed sets* and *sijections*, signed bijections between signed sets. We present the basic concepts here, and refer the reader to [14, §2] for all the details and more examples.

A *signed set* is a pair of disjoint finite sets: $\underline{S} = (S^+, S^-)$ with $S^+ \cap S^- = \varnothing$. Equivalently, a signed set is a finite set S together with a sign function $\operatorname{sign}\colon S \to \{1, -1\}$, but we will mostly avoid the use of the sign function. Signed sets are usually underlined throughout the extended abstract with the following exception: an ordinary set S always induces a signed set $\underline{S} = (S, \varnothing)$, and in this case we identify $\underline{S}$ with S. We summarize related notions.

- The *size* of a signed set $\underline{S}$ is $|\underline{S}| = |S^+| - |S^-|$.
- The *opposite* signed set of $\underline{S}$ is $-\underline{S} = (S^-, S^+)$.
- The *Cartesian product* of signed sets $\underline{S}$ and $\underline{T}$ is $\underline{S} \times \underline{T} = (S^+ \times T^+ \cup S^- \times T^-, S^+ \times T^- \cup S^- \times T^+)$.
- The *disjoint union* of signed sets $\underline{S}$ and $\underline{T}$ is $\underline{S} \sqcup \underline{T} = (\underline{S} \times (\{0\}, \varnothing)) \cup (\underline{T} \times (\{1\}, \varnothing))$. The *disjoint union of a family of signed sets $\underline{S}_t$* indexed with a signed set $\underline{T}$ is

  $$\bigsqcup_{t \in \underline{T}} \underline{S}_t = \bigcup_{t \in \underline{T}} (\underline{S}_t \times \underline{\{t\}}).$$

  Here $\underline{\{t\}}$ is $(\{t\}, \varnothing)$ if $t \in T^+$ and $(\varnothing, \{t\})$ if $t \in T^-$.

[1] The code (in python) is available at `https://www.fmf.uni-lj.si/~konvalinka/asmcode.html`.

Most of the usual properties of Cartesian products and disjoint unions of ordinary sets extend to signed sets.

An important type of signed sets are signed intervals: for $a, b \in \mathbb{Z}$, define

$$\underline{[a,b]} = \begin{cases} ([a,b], \varnothing) & \text{if } a \le b \\ (\varnothing, [b+1, a-1]) & \text{if } a > b \end{cases}.$$

Here $[a,b]$ stands for the usual interval in $\mathbb{Z}$. The signed sets that are of relevance in this extended abstract are usually constructed from signed intervals using Cartesian products and disjoint unions.

The role of bijections for signed sets is played by "signed bijections", which we call *sijections*. A sijection φ from $\underline{S}$ to $\underline{T}$,

$$\varphi \colon \underline{S} \Rightarrow \underline{T},$$

is an involution on the set $(S^+ \cup S^-) \sqcup (T^+ \cup T^-)$ with the property $\varphi(S^+ \sqcup T^-) = S^- \sqcup T^+$. It follows that also $\varphi(S^- \sqcup T^+) = S^+ \sqcup T^-$. A sijection can also be thought of as a collection of a sign-reversing involution on a subset of $\underline{S}$, a sign-reversing involution on a subset of $\underline{T}$, and a sign-preserving matching between the remaining elements of $\underline{S}$ with the remaining elements of $\underline{T}$. The existence of a sijection $\varphi \colon \underline{S} \Rightarrow \underline{T}$ clearly implies $|\underline{S}| = |S^+| - |S^-| = |T^+| - |T^-| = |\underline{T}|$.

In Proposition 2 of [14] it is explained how to construct the Cartesian product and the disjoint union of sijections, and also how to compose two sijections using a variant of the Garsia-Milne involution principle. These constructions are fundamental for most of the constructions in this extended abstract. It follows that the existence of a sijection between $\underline{S}$ and $\underline{T}$ is an equivalence relation; it is denoted by "$\approx$".

The sijection that is underlying many of our constructions is the following.

▶ **Problem 3** ([14, Problem 1]). *Given $a, b, c \in \mathbb{Z}$, construct a sijection*

$$\alpha = \alpha_{a,b,c} \colon \underline{[a,c]} \Longrightarrow \underline{[a,b]} \sqcup \underline{[b+1,c]} = \underline{[a,b]} \sqcup -\underline{[c+1,b]}.$$

Construction. For $a \le b \le c$ and $c < b < a$, there is nothing to prove. For, say, $a \le c < b$, we have $\underline{[a,b]} \sqcup \underline{[b+1,c]} = (\underline{[a,c]} \sqcup \underline{[c+1,b]}) \sqcup \underline{[b+1,c]} = \underline{[a,c]} \sqcup (\underline{[c+1,b]} \sqcup (-\underline{[c+1,b]}))$. Since there is a sijection $\underline{[c+1,b]} \sqcup (-\underline{[c+1,b]}) \Rightarrow \underline{\varnothing}$, we get a sijection $\underline{[a,b]} \sqcup \underline{[b+1,c]} \Rightarrow \underline{[a,c]}$. The cases $b < a \le c$, $b \le c < a$, and $c < a \le b$ are analogous. ◀

Using the map α, it is not difficult to construct some sijections on *signed boxes*, Cartesian products of signed intervals. We sketch two such constructions (for the following problem, and for the related Problem 6), and state other necessary results. The first construction is related to Lemma 2.2 in [13], which plays a crucial role in the non-bijective proof that was the starting point for our constructions. Also in the following we indicate such relations whenever it is possible.

▶ **Problem 4** ([14, Problem 2]). *Given $\mathbf{a} = (a_1, \dots, a_{n-1}) \in \mathbb{Z}^{n-1}$, $\mathbf{b} = (b_1, \dots, b_{n-1}) \in \mathbb{Z}^{n-1}$, $x \in \mathbb{Z}$, write $\underline{S}_i = (\{a_i\}, \varnothing) \sqcup (\varnothing, \{b_i + 1\})$, and construct a sijection*

$$\beta = \beta_{\mathbf{a},\mathbf{b},x} \colon \underline{[a_1,b_1]} \times \cdots \times \underline{[a_{n-1},b_{n-1}]} \\ \Longrightarrow \bigsqcup_{(l_1,\dots,l_{n-1}) \in \underline{S}_1 \times \cdots \times \underline{S}_{n-1}} \underline{[l_1,l_2]} \times \underline{[l_2,l_3]} \times \cdots \times \underline{[l_{n-2},l_{n-1}]} \times \underline{[l_{n-1},x]}.$$

Construction. The proof is by induction, with the case $n = 1$ being trivial and the case $n = 2$ was constructed in Problem 3. Now, for $n \geq 3$,

$$\begin{aligned}
&\underline{[a_1, b_1]} \times \cdots \times \underline{[a_{n-1}, b_{n-1}]} \approx \underline{[a_1, b_1]} \times \bigsqcup_{(l_2,\dots,l_{n-1}) \in \underline{S}_2 \times \cdots \times \underline{S}_{n-1}} \underline{[l_2, l_3]} \times \cdots \times \underline{[l_{n-2}, l_{n-1}]} \times \underline{[l_{n-1}, x]} \\
&\approx \left(\underline{[a_1, b_1]} \times \bigsqcup_{(l_3,\dots,l_{n-1}) \in \underline{S}_3 \times \cdots \times \underline{S}_{n-1}} \underline{[a_2, l_3]} \times \cdots \times \underline{[l_{n-1}, x]} \right) \\
&\qquad \sqcup \left(\underline{[a_1, b_1]} \times \bigsqcup_{(l_3,\dots,l_{n-1}) \in \underline{S}_3 \times \cdots \times \underline{S}_{n-1}} (-\underline{[b_2 + 1, l_3]}) \times \cdots \times \underline{[l_{n-1}, x]} \right),
\end{aligned}$$

where we used induction for the first equivalence, and distributivity and the fact that $S_2 = (\{a_2\}, \varnothing) \sqcup (\varnothing, \{b_2 + 1\})$ for the second equivalence. By Problem 3 and standard sijection constructions, there exists a sijection from the last expression to

$$\begin{aligned}
&\left(\left(\underline{[a_1, a_2]} \sqcup (-\underline{[b_1 + 1, a_2]}) \right) \times \bigsqcup_{(l_3,\dots,l_{n-1}) \in \underline{S}_3 \times \cdots \times \underline{S}_{n-1}} \underline{[a_2, l_3]} \times \cdots \times \underline{[l_{n-1}, x]} \right) \\
&\sqcup \left(\left(\underline{[a_1, b_2 + 1]} \sqcup (-\underline{[b_1 + 1, b_2 + 1]}) \right) \times \bigsqcup_{(l_3,\dots,l_{n-1}) \in \underline{S}_3 \times \cdots \times \underline{S}_{n-1}} (-\underline{[b_2 + 1, l_3]}) \times \cdots \times \underline{[l_{n-1}, x]} \right) \\
&\qquad \approx \bigsqcup_{(l_1,\dots,l_{n-1}) \in \underline{S}_1 \times \cdots \times \underline{S}_{n-1}} \underline{[l_1, l_2]} \times \underline{[l_2, l_3]} \times \cdots \cdots \underline{[l_{n-2}, l_{n-1}]} \times \underline{[l_{n-1}, x]},
\end{aligned}$$

where for the last equivalence we have again used distributivity. ◀

▶ **Problem 5** ([14, Problem 3]). *Given* $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{Z}^n$ *and* $x \in \mathbb{Z}$, *construct a sijection*

$$\begin{aligned}
&\gamma = \gamma_{\mathbf{k},x} \colon \underline{[k_1, k_2]} \times \cdots \times \underline{[k_{n-1}, k_n]} \\
&\Longrightarrow \bigsqcup_{i=1}^{n} \underline{[k_1, k_2]} \times \cdots \times \underline{[k_{i-1}, x + n - i]} \times \underline{[x + n - i, k_{i+1}]} \times \cdots \times \underline{[k_{n-1}, k_n]} \\
&\quad \sqcup \bigsqcup_{i=1}^{n-2} \cdots \times \underline{[k_{i-1}, k_i]} \times \underline{[k_{i+1} + 1, x + n - i - 1]} \times \underline{[k_{i+1}, x + n - i - 2]} \times \underline{[k_{i+2}, k_{i+3}]} \times \cdots .
\end{aligned}$$

An important signed set is the set of all Gelfand-Tsetlin patterns, or GT patterns for short (compare with [10]), with a prescribed bottom row. For $k \in \mathbb{Z}$, define $\underline{\mathrm{GT}}(k) = (\{\cdot\}, \varnothing)$,[2] and for $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{Z}^n$, define recursively

$$\underline{\mathrm{GT}}(\mathbf{k}) = \underline{\mathrm{GT}}(k_1, \dots, k_n) = \bigsqcup_{\mathbf{l} \in \underline{[k_1, k_2]} \times \cdots \times \underline{[k_{n-1}, k_n]}} \underline{\mathrm{GT}}(l_1, \dots, l_{n-1}).$$

In particular, $\underline{\mathrm{GT}}(a, b) \approx \underline{[a, b]}$. One can think of an element of $\underline{\mathrm{GT}}(\mathbf{k})$ as a triangular array $A = (A_{i,j})_{1 \leq j \leq i \leq n}$

$$\begin{array}{ccccccccc}
 & & & & A_{1,1} & & & & \\
 & & & A_{2,1} & & A_{2,2} & & & \\
 & & A_{3,1} & & A_{3,2} & & A_{3,3} & & \\
 & \iddots & \vdots & \ddots & \vdots & \iddots & \vdots & \ddots & \\
A_{n,1} & & A_{n,2} & & \dots & & \dots & & A_{n,n},
\end{array}$$

so that $A_{i+1,j} \leq A_{i,j} \leq A_{i+1,j+1}$ or $A_{i+1,j} > A_{i,j} > A_{i+1,j+1}$ for $1 \leq j \leq i < n$, and $A_{n,i} = k_i$.

---

[2] Instead of $\{\cdot\}$, one can take any one-element set.

The following sijections are crucial for GT patterns. In the constructions, we typically use disjoint unions of previously constructed sijections on signed boxes (e.g. Problem 4).

▶ **Problem 6** ([14, Problem 4]). *Given* $\mathbf{a} = (a_1, \ldots, a_{n-1}) \in \mathbb{Z}^{n-1}$*,* $\mathbf{b} = (b_1, \ldots, b_{n-1}) \in \mathbb{Z}^{n-1}$*,* $x \in \mathbb{Z}$*, construct a sijection*

$$\rho = \rho_{\mathbf{a},\mathbf{b},x}\colon \bigsqcup_{\mathbf{l} \in \underline{[a_1,b_1]} \times \cdots \times \underline{[a_{n-1},b_{n-1}]}} \underline{\mathrm{GT}}(\mathbf{l}) \Rightarrow \bigsqcup_{(l_1,\ldots,l_{n-1}) \in \underline{S}_1 \times \cdots \times \underline{S}_{n-1}} \underline{\mathrm{GT}}(l_1, \ldots, l_{n-1}, x),$$

where $\underline{S}_i = (\{a_i\}, \emptyset) \sqcup (\emptyset, \{b_i + 1\})$.

Construction. In Problem 4, we constructed a sijection

$$\underline{[a_1, b_1]} \times \cdots \times \underline{[a_{n-1}, b_{n-1}]} \Rightarrow \bigsqcup_{(l_1,\ldots,l_{n-1}) \in \underline{S}_1 \times \cdots \times \underline{S}_{n-1}} \underline{[l_1, l_2]} \times \underline{[l_2, l_3]} \times \cdots \times \underline{[l_{n-2}, l_{n-1}]} \times \underline{[l_{n-1}, x]}.$$

By standard sijection constructions, this gives a sijection

$$\bigsqcup_{\mathbf{l} \in \underline{[a_1,b_1]} \times \cdots \times \underline{[a_{n-1},b_{n-1}]}} \underline{\mathrm{GT}}(\mathbf{l}) \Rightarrow \bigsqcup_{\mathbf{m} \in \bigsqcup_{(l_1,\ldots,l_{n-1}) \in \underline{S}_1 \times \cdots \times \underline{S}_{n-1}} \underline{[l_1,l_2]} \times \underline{[l_2,l_3]} \times \cdots \times \underline{[l_{n-2},l_{n-1}]} \times \underline{[l_{n-1},x]}} \underline{\mathrm{GT}}(\mathbf{m}).$$

This is equivalent to

$$\bigsqcup_{(l_1,\ldots,l_{n-1}) \in \underline{S}_1 \times \cdots \times \underline{S}_{n-1}} \; \bigsqcup_{\mathbf{m} \in \underline{[l_1,l_2]} \times \underline{[l_2,l_3]} \times \cdots \times \underline{[l_{n-2},l_{n-1}]} \times \underline{[l_{n-1},x]}} \underline{\mathrm{GT}}(\mathbf{m}),$$

and by definition of $\underline{\mathrm{GT}}$, this is equal to $\bigsqcup_{(l_1,\ldots,l_{n-1}) \in \underline{S}_1 \times \cdots \times \underline{S}_{n-1}} \underline{\mathrm{GT}}(l_1, \ldots, l_{n-1}, x)$. ◀

The result is important because while it adds a dimension to GT patterns, it (typically) greatly reduces the size of the indexing signed set. In fact, there is an analogy to the fundamental theorem of calculus: instead of extending the disjoint union over the entire signed box, it suffices to consider the boundary; x corresponds in a sense to the constant of integration.

▶ **Problem 7** ([14, Problem 5]). *Given* $\mathbf{k} = (k_1, \ldots, k_n) \in \mathbb{Z}^n$ *and* i*,* $1 \le i \le n-1$*, construct a sijection*

$$\pi = \pi_{\mathbf{k},i}\colon \underline{\mathrm{GT}}(k_1, \ldots, k_n) \Rightarrow -\underline{\mathrm{GT}}(k_1, \ldots, k_{i-1}, k_{i+1} + 1, k_i - 1, k_{i+2}, \ldots, k_n).$$

Given $\mathbf{a} = (a_1, \ldots, a_n) \in \mathbb{Z}^n$*,* $\mathbf{b} = (b_1, \ldots, b_n) \in \mathbb{Z}^n$ *such that for some* i*,* $1 \le i \le n-1$*, we have* $a_{i+1} = a_i - 1$ *and* $b_{i+1} = b_i - 1$*, construct a sijection*

$$\sigma = \sigma_{\mathbf{a},\mathbf{b},i}\colon \bigsqcup_{\mathbf{l} \in \underline{[a_1,b_1]} \times \cdots \times \underline{[a_n,b_n]}} \underline{\mathrm{GT}}(\mathbf{l}) \Rightarrow \underline{\emptyset}.$$

The reason we place these two sijections in the same problem is that the proof is by induction, with the induction step for π using σ and vice versa.

▶ **Problem 8** ([14, Problem 6]). *Given* $\mathbf{k} = (k_1, \ldots, k_n) \in \mathbb{Z}^n$ *and* $x \in \mathbb{Z}$*, construct a sijection*

$$\tau = \tau_{\mathbf{k},x}\colon \underline{\mathrm{GT}}(k_1, \ldots, k_n) \Rightarrow \bigsqcup_{i=1}^{n} \underline{\mathrm{GT}}(k_1, \ldots, k_{i-1}, x + n - i, k_{i+1}, \ldots, k_n).$$

3 Monotone triangles and the operator formula

Monotone triangles with bottom row $1, 2, \dots, n$ are in easy bijective correspondence with $n \times n$ alternating sign matrices. For our purpose we need to have a notion of monotone triangles with arbitrary integer bottom rows. In order to achieve this, suppose that $\mathbf{k} = (k_1, \dots, k_n)$ and $\mathbf{l} = (l_1, \dots, l_{n-1})$ are two sequences of integers. We say that $\mathbf{l}$ *interlaces* $\mathbf{k}$, $\mathbf{l} \prec \mathbf{k}$, if the following holds:

1. for every i, $1 \le i \le n-1$, l_i is in the closed interval between k_i and k_{i+1};
2. if $k_{i-1} \le k_i \le k_{i+1}$ for some i, $2 \le i \le n-1$, then l_{i-1} and l_i cannot both be k_i;
3. if $k_i > l_i = k_{i+1}$, then $i \le n-2$ and $l_{i+1} = l_i = k_{i+1}$;
4. if $k_i = l_i > k_{i+1}$, then $i \ge 2$ and $l_{i-1} = l_i = k_i$.

A *monotone triangle of size* n is a map $T\colon \{(i,j)\colon 1 \le j \le i \le n\} \to \mathbb{Z}$ so that line $i-1$ (i.e. the sequence $T_{i-1,1}, \dots, T_{i-1,i-1}$) interlaces line i (i.e. the sequence $T_{i,1}, \dots, T_{i,i}$). The *sign* of a monotone triangle T is $(-1)^r$, where r is the sum of:

- the number of strict descents in the rows of T, i.e. the number of pairs (i,j) so that $1 \le j < i \le n$ and $T_{i,j} > T_{i,j+1}$, and
- the number of (i,j) so that $1 \le j \le i-2$, $i \le n$ and $T_{i,j} > T_{i-1,j} = T_{i,j+1} = T_{i-1,j+1} > T_{i,j+2}$.

It turns out that $\underline{\mathrm{MT}}(\mathbf{k})$ satisfies a recursive "identity". Let us define the signed set of *arrow rows of order* n as $\underline{\mathrm{AR}}_n = (\{\nearrow, \nwarrow\}, \{\nwarrow\!\!\!\!\nearrow\})^n$. The role of an arrow row μ of order n is that it induces a deformation of $\underline{[k_1, k_2]} \times \underline{[k_2, k_3]} \times \cdots \times \underline{[k_{n-1}, k_n]}$ as follows. Consider

$$\begin{array}{ccccccccc} & \underline{[k_1,k_2]} & & \underline{[k_2,k_3]} & & \dots & \underline{[k_{n-2},k_n-1]} & & \underline{[k_{n-1},k_n]} & \\ \mu_1 & & \mu_2 & & \mu_3 & \dots & & \mu_{n-1} & & \mu_n, \end{array}$$

and if $\mu_i \in \{\nwarrow, \nwarrow\!\!\!\!\nearrow\}$ (that is we have an arrow pointing towards $\underline{[k_{i-1}, k_i]}$) then k_i is decreased by 1 in $\underline{[k_{i-1}, k_i]}$, while there is no change for this k_i if $\mu_i = \nearrow$. If $\mu_i \in \{\nearrow, \nwarrow\!\!\!\!\nearrow\}$ then k_i is increased by 1 in $[k_i, k_{i+1}]$, while there is no change for this k_i if $\mu_i = \nwarrow$. For a more formal description, we let $\delta_{\nwarrow}(\nwarrow) = \delta_{\nwarrow}(\nwarrow\!\!\!\!\nearrow) = \delta_{\nearrow}(\nearrow) = \delta_{\nearrow}(\nwarrow\!\!\!\!\nearrow) = 1$ and $\delta_{\nwarrow}(\nearrow) = \delta_{\nearrow}(\nwarrow) = 0$, and we define

$$e(\mathbf{k}, \mu) = \underline{[k_1 + \delta_{\nearrow}(\mu_1), k_2 - \delta_{\nwarrow}(\mu_2)]} \times \dots \times \underline{[k_{n-1} + \delta_{\nearrow}(\mu_{n-1}), k_n - \delta_{\nwarrow}(\mu_n)]}.$$

for $\mathbf{k} = (k_1, \dots, k_n)$ and $\mu \in \underline{\mathrm{AR}}_n$. The following is not difficult.

▶ **Problem 9** ([14, Problem 7]). *Given* $\mathbf{k} = (k_1, \dots, k_n)$, *construct a sijection*

$$\Xi = \Xi_{\mathbf{k}} \colon \underline{\mathrm{MT}}(\mathbf{k}) \Rightarrow \bigsqcup_{\mu \in \underline{\mathrm{AR}}_n} \bigsqcup_{\mathbf{l} \in e(\mathbf{k},\mu)} \underline{\mathrm{MT}}(\mathbf{l}).$$

Our next goal is to define other objects that satisfy the same "recursion" as monotone triangles. To this end, define the signed set of *arrow patterns of order* n as

$$\underline{\mathrm{AP}}_n = (\{\swarrow, \searrow\}, \{\swarrow\!\!\!\!\searrow\})^{\binom{n}{2}}.$$

Alternatively, we can think of an arrow pattern of order n as a triangular array $T = (t_{p,q})_{1 \le p < q \le n}$ arranged as

$$T = \begin{array}{ccccccccc} & & & & t_{1,n} & & & & \\ & & & t_{1,n-1} & & t_{2,n} & & & \\ & & t_{1,n-2} & & t_{2,n-1} & & t_{3,n} & & \\ & \cdot^{\cdot^{\cdot}} & \vdots & \ddots & \vdots & \cdot^{\cdot^{\cdot}} & \vdots & \ddots & \\ t_{1,2} & & t_{2,3} & & \dots & & \dots & & t_{n-1,n} \end{array},$$

with $t_{p,q} \in \{\swarrow, \searrow, \swarrow\!\!\!\!\searrow\}$, and the sign of an arrow pattern is 1 if the number of $\swarrow\!\!\!\!\searrow$'s is even and -1 otherwise.

The role of an arrow pattern of order n is that it induces a deformation of $(k_1, \dots, k_n)$, which can be thought of as follows. Add $k_1, \dots, k_n$ as bottom row of T (i.e., $t_{i,i} = k_i$), and for each $\swarrow$ or $\swarrow\!\!\!\!\searrow$ which is in the same $\swarrow$-diagonal as k_i add 1 to k_i, while for each $\searrow$ or $\swarrow\!\!\!\!\searrow$ which is in the same $\searrow$-diagonal as k_i subtract 1 from k_i. More formally, letting $\delta_{\swarrow}(\swarrow) = \delta_{\swarrow}(\swarrow\!\!\!\!\searrow) = \delta_{\searrow}(\searrow) = \delta_{\searrow}(\swarrow\!\!\!\!\searrow) = 1$ and $\delta_{\swarrow}(\searrow) = \delta_{\searrow}(\swarrow) = 0$, we set

$$c_i(T) = \sum_{j=i+1}^{n} \delta_{\swarrow}(t_{i,j}) - \sum_{j=1}^{i-1} \delta_{\searrow}(t_{j,i}) \text{ and } d(\mathbf{k}, T) = (k_1 + c_1(T), k_2 + c_2(T), \dots, k_n + c_n(T))$$

for $\mathbf{k} = (k_1, \dots, k_n)$ and $T \in \underline{\mathrm{AP}}_n$.

For $\mathbf{k} = (k_1, \dots, k_n)$ define *shifted Gelfand-Tsetlin patterns*, or SGT patterns for short, as the following disjoint union of GT patterns over arrow patterns of order n:

$$\underline{\mathrm{SGT}}(\mathbf{k}) = \bigsqcup_{T \in \underline{\mathrm{AP}}_n} \underline{\mathrm{GT}}(d(\mathbf{k}, T))$$

The difficult part of [14] is to prove that $\underline{\mathrm{SGT}}$ indeed satisfies the same "recursion" as $\underline{\mathrm{MT}}$. While the proof of the recursion was easy for monotone triangles, it is very involved for shifted GT patterns, and needs almost all the sijections we have mentioned so far.

▶ **Problem 10** ([14, Problem 9]). *Given* $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{Z}^n$ *and* $x \in \mathbb{Z}$, *construct a sijection*

$$\Phi = \Phi_{\mathbf{k},x} \colon \bigsqcup_{\mu \in \underline{\mathrm{AR}}_n} \bigsqcup_{\mathbf{l} \in e(\mathbf{k},\mu)} \underline{\mathrm{SGT}}(\mathbf{l}) \Rightarrow \underline{\mathrm{SGT}}(\mathbf{k}).$$

From the last problem, it is easy to construct a bijective proof of the operator formula for monotone triangles. See [14, pp. 3–4] for a discussion of this formula.

▶ **Problem 11** ([14, Problem 10]). *Given* $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{Z}^n$ *and* $x \in \mathbb{Z}$, *construct a sijection*

$$\Gamma = \Gamma_{\mathbf{k},x} \colon \underline{\mathrm{MT}}(\mathbf{k}) \Rightarrow \underline{\mathrm{SGT}}(\mathbf{k}).$$

Construction. The proof is by induction on n. For $n = 1$, both sides consist of one (positive) element, and the sijection is obvious. Once we have constructed Γ for all lists of length less than n, we can construct $\Gamma_{\mathbf{k},x}$ as the composition of sijections

$$\underline{\mathrm{MT}}(\mathbf{k}) \xRightarrow{\Xi_{\mathbf{k}}} \bigsqcup_{\mu \in \underline{\mathrm{AR}}_n} \bigsqcup_{\mathbf{l} \in e(\mathbf{k},\mu)} \underline{\mathrm{MT}}(\mathbf{l}) \xRightarrow{\sqcup\sqcup\Gamma} \bigsqcup_{\mu \in \underline{\mathrm{AR}}_n} \bigsqcup_{\mathbf{l} \in e(\mathbf{k},\mu)} \underline{\mathrm{SGT}}(\mathbf{l}) \xRightarrow{\Phi_{\mathbf{k},x}} \underline{\mathrm{SGT}}(\mathbf{k}),$$

where $\sqcup \sqcup \Gamma$ means $\bigsqcup_{\mu \in \underline{\mathrm{AR}}_n} \bigsqcup_{\mathbf{l} \in e(\mathbf{k},\mu)} \Gamma_{\mathbf{l},x}$. ◀

4 Sketch of the main bijections

Equipped with the operator formula, one can construct the following crucial sijection. (This corresponds to Theorem 2.4 in the non-bijective proof in [13].)

▶ **Problem 12** ([15, Problem 16]). *Given* $\mathbf{k} = (k_1, \dots, k_n)$, *construct a sijection*

$$\underline{\mathrm{MT}}(\mathbf{k}) \Longrightarrow (-1)^{n-1}\, \underline{\mathrm{MT}}(\mathrm{rot}(\mathbf{k})),$$

where $\mathrm{rot}(\mathbf{k}) = (k_2, \dots, k_n, k_1 - n)$.

Note that the construction is far from easy, even assuming that we have the map Γ. See [15, §6] for a proof. On the other hand, the following is relatively simple.

Suppose that we are given a weakly increasing sequence $\mathbf{k} = (k_1, \dots, k_n)$ and $i \in \mathbb{N}$. We define

$$\underline{\mathrm{MT}}_i(\mathbf{k}) = \{T \in \underline{\mathrm{MT}}(\mathbf{k}) \colon T_{n-i+1,1} = \dots = T_{n,1} = k_1, T_{n-i,1} \neq k_1\}$$

as the signed subset of monotone triangles with k_1 in the first position in exactly the last i rows. Similarly, we define

$$\underline{\mathrm{MT}}^i(\mathbf{k}) = \{T \in \underline{\mathrm{MT}}(\mathbf{k}) \colon T_{n-i+1,n-i+1} = \dots = T_{n,n} = k_n, T_{n-i,n-i} \neq k_n\}$$

as the signed subset of monotone triangles with k_n in the last position in exactly the last i rows.

The following corresponds to Proposition 2.6 in [13].

▶ **Problem 13** ([15, Problem 21]). *Given a weakly increasing* $\mathbf{k} = (k_1, \dots, k_n)$ *and* $i \geq 1$, *construct sijections*

$$\underline{\mathrm{MT}}_i(\mathbf{k}) \Longrightarrow \bigsqcup_{j=0}^{i-1} (-1)^j \binom{[i-1]}{j} \times \underline{\mathrm{MT}}(k_1 + j + 1, k_2, \dots, k_n)$$

and

$$\underline{\mathrm{MT}}^i(\mathbf{k}) \Longrightarrow \bigsqcup_{j=0}^{i-1} (-1)^j \binom{[i-1]}{j} \times \underline{\mathrm{MT}}(k_1, k_2, \dots, k_n - j - 1).$$

Based on the last two constructions, it is quite straightforward to do the following. It corresponds to Proposition 2.7 in [13].

▶ **Problem 14** ([15, Problem 22]). *Given* $n \in \mathbb{N}$ *and* $i \in [n]$, *construct a sijection*

$$\bigsqcup_{j=1}^{n} (-1)^{j+1} \binom{[2n-i-1]}{n-i-j+1} \times \mathrm{ASM}_{n,j} \Longrightarrow \mathrm{ASM}_{n,i}\,.$$

To complete the construction of the bijections for Problems 1 and 2, we need, among other results, a few more ingredients from "bijective linear algebra". Denote by $\underline{\mathfrak{S}}_m$ the signed set of permutations (with the usual sign). Given signed sets $\underline{P}_{i,j}$, $1 \leq i, j \leq m$, define the *determinant* of $\underline{\mathcal{P}} = [\underline{P}_{ij}]_{i,j=1}^m$ as the signed set

$$\det(\underline{\mathcal{P}}) = \bigsqcup_{\pi \in \underline{\mathfrak{S}}_m} \underline{P}_{1,\pi(1)} \times \cdots \times \underline{P}_{m,\pi(m)}.$$

Among other classical properties, we have the following version of Cramer's rule.

▶ **Problem 15** ([15, Problem 9]). *Given* $\underline{\mathcal{P}} = [\underline{P}_{p,q}]_{p,q=1}^m$, *signed sets* $\underline{X}_i, \underline{Y}_i$ *and sijections* $\bigsqcup_{q=1}^m \underline{P}_{i,q} \times \underline{X}_q \Rightarrow \underline{Y}_i$ *for all* $i \in [m]$, *construct sijections*

$$\det(\underline{\mathcal{P}}) \times \underline{X}_j \Longrightarrow \det(\underline{\mathcal{P}}^j),$$

where $\underline{\mathcal{P}}^j = [\underline{P}^j_{p,q}]_{p,q=1}^m$, $\underline{P}^j_{p,q} = \underline{P}_{p,q}$ *if* $q \neq j$, $\underline{P}^j_{p,j} = \underline{Y}_p$, *for all* $j \in [m]$.

Essentially, sijections like the one in Problem 15 tell us that "linear equalities" for sijections like the one in Problem 14 can be used to find bijections on the sets involved. See the constructions for Problems 1 and 2 in [15, §7] for all details.

5 Summary

In this extended abstract, we present the first bijective proof of the enumeration formula for alternating sign matrices. The bijection is by no means simple; the papers [14, 15] combined have about 40 pages, with the technical constructions taking about 20 pages. We also needed more than 2000 lines to produce a working python code. However, note that the first proof of the ASM theorem by Zeilberger was 84 pages long. We certainly hope that our proof will be simplified and shortened in the future.

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Counting Cubic Maps with Large Genus

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Abstract

We derive an asymptotic expression for the number of cubic maps on orientable surfaces when the genus is proportional to the number of vertices. Let Σ_g denote the orientable surface of genus g and $\theta = g/n \in (0, 1/2)$. Given $g, n \in \mathbb{N}$ with $g \to \infty$ and $\frac{n}{2} - g \to \infty$ as $n \to \infty$, the number $C_{n,g}$ of cubic maps on Σ_g with $2n$ vertices satisfies

$$C_{n,g} \;\sim\; (g!)^2\, \alpha(\theta)\, \beta(\theta)^n\, \gamma(\theta)^{2g}, \quad \text{as} \quad g \to \infty,$$

where $\alpha(\theta), \beta(\theta), \gamma(\theta)$ are differentiable functions in $(0, 1/2)$. This also leads to the asymptotic number of triangulations (as the dual of cubic maps) with large genus. When g/n lies in a closed subinterval of $(0, 1/2)$, the asymptotic formula can be obtained using a local limit theorem. The saddle-point method is applied when $g/n \to 0$ or $g/n \to 1/2$.

2012 ACM Subject Classification Mathematics of computing → Generating functions; Mathematics of computing → Enumeration

Keywords and phrases cubic maps, triangulations, cubic graphs on surfaces, generating functions, asymptotic enumeration, local limit theorem, saddle-point method

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.13

Funding *Zhicheng Gao*: Research supported by NSERC.
Mihyun Kang: Research supported by the Austrian Science Fund (FWF): I3747, W1230.

Acknowledgements Part of this research was carried out while the first author was visiting TU Graz. This visit was financially supported by TU Graz within the Doctoral Program "Discrete Mathematics".

1 Introduction

Since the seminal work of Tutte on planar maps [19], various types of maps on surfaces have attracted much attention (see e.g. [3, 4, 11, 13]). Most of results on maps deal with the case when the genus is *constant*. When the genus is proportional to the number of vertices, edges or faces, there are only a few results, which deal with either maps with one face (also known as unicellular maps) [1, 7, 18] or triangular maps (also known as triangulations) [6].

In this paper we study cubic maps (and their dual, triangular maps) on orientable surfaces of non-constant genus. As demonstrated in [8, 15], such cubic maps form base cases in the study of sparse random graphs of non-constant genus. Furthermore, the study of random graphs of non-constant genus has only been initiated very recently [8, 16], and it is likely to prove to be the most interesting – the "evolution" of random graphs of non-constant genus depends heavily on the ratios between the genus, the number of edges, and the number of vertices, and it "transforms" from a random forest to the classical Erdős-Rény random graph.

We let Σ_g denote the orientable surface of genus g. A map on Σ_g is a connected graph G that is *embedded* on Σ_g in such a way that each component of $\Sigma_g - G$, called *a face*, is simply connected region. A map on Σ_g will be called a map with genus g. Throughout the paper, a map is always *rooted*, meaning that an edge is distinguished together with an end vertex and a side of it.

A map is called *cubic* if all its vertices have degree 3. The dual of a cubic map is called a *triangular map* whose faces all have degree 3. Let $C_{n,g}$ be the number of cubic maps with $2n$ vertices and genus g and $T_{n,g}$ be the number of triangular maps with n vertices and genus g. Recall Euler's formula for a map with v vertices, e edges, f faces, and genus g:

$$v - e + f = 2 - 2g.$$

In addition, a triangular map with e edges and f faces satisfies $2e = 3f$, and therefore a triangular map with v vertices and genus g has exactly $2(v + 2g - 2)$ faces, which in dual corresponds to a cubic map with $2(v + 2g - 2)$ vertices and genus g. Thus, we have

$$C_{n,g} \;=\; T_{n-2g+2,g}. \tag{1}$$

A direct consequence is that there are no cubic maps on Σ_g with $2n$ vertices (and hence $C_{n,g} = 0$), if $2g > n + 1$. Therefore, throughout the paper we assume $2g \le n + 1$.

When g is *constant*, the following asymptotic formulas for $T_{n,g}$ and $C_{n,g}$ were determined by Gao [10]: as $n \to \infty$,

$$C_{n,g} \;\sim\; 3 \cdot 6^{(g-1)/2}\, t_g\, n^{5(g-1)/2}\, (12\sqrt{3})^n, \tag{2}$$

$$T_{n,g} \;\sim\; 3 \cdot (2^9 \cdot 3^7)^{(g-1)/2}\, t_g\, n^{5(g-1)/2}\, (12\sqrt{3})^n. \tag{3}$$

In fact, the constant t_g appears universally in the asymptotic formulas for various rooted maps on Σ_g [3, 4, 11, 13]. Its asymptotic expression was derived by Bender, Gao, and Richmond [5]:

$$t_g \;\sim\; \frac{10\,(3/5)^{1/2}\,\Gamma(1/5)\,\Gamma(4/5)\,\sin(\pi/5)}{2^{1/2}\,\pi^{5/2}} \left(\frac{1440\,g}{e}\right)^{-g/2}, \quad \text{as} \quad g \to \infty. \tag{4}$$

In this paper we study cubic maps on Σ_g when g is *non-constant*, particularly when $g/n \in (0, 1/2)$. We determine the asymptotic behavior of the generating function for $C_{n,g}$ (Theorem 1) and an asymptotic expression for $C_{n,g}$ (Theorems 2 and 3) as $g \to \infty$ and $n - 2g \to \infty$.

Following the notation in [5] we let $C_g(x) := \sum_{n \ge 0} C_{n,g} x^n$ denote the generating function for cubic maps on Σ_g. The parametrization given by (15) in [5]

$$x \;=\; \frac{1}{12\sqrt{3}}(1-s)\sqrt{1+2s} \quad (0 < s < 1)$$

was quite useful when the genus g is constant. However, in order to study the asymptotic behaviors of $C_g(x)$ and $C_{n,g}$ for *non-constant* genus g satisfying $g/n \in (0, 1/2)$, it turns out to be more convenient to use the following parametrization

$$x(t) := \;\frac{t}{4}(1+2t)^{-3/2}. \tag{5}$$

Note that $x(t)$ is monotonically increasing in $t \in [0, 1]$. In addition, we define functions θ, r, A, σ^2 in $t \in (0, 1)$ by

$$\theta(t) := \frac{1}{2} - \frac{3t}{4(1+2t)\sqrt{1-t}} \ln \frac{1+\sqrt{1-t}}{1-\sqrt{1-t}}, \tag{6}$$

$$r(t) := \frac{2(1+2t)\sqrt{1-t}}{3t}\theta(t), \tag{7}$$

$$\sigma^2(t) := \frac{1}{2\theta^2(t)} - \frac{2t^2-t+2}{2(1-t)^2\theta(t)}, \tag{8}$$

$$A(t) := \frac{27K}{8}(1+2t)^{-1/2}\left(\frac{t}{2(1-t)\theta(t)}\right)^{3/2}, \tag{9}$$

where $K \doteq 1.2 \times 10^{-6}$ is some positive constant.

Our first main result is the following asymptotic expression for $C_g(x)$.

▶ **Theorem 1.** *Let x be on the complex plane. Uniformly for $|x|$ in any given closed subinterval of $\big(0, 1/(12\sqrt{3})\big)$, the generating function $C_g(x)$ for cubic maps with genus g satisfies*

$$C_g(x) \;=\; C_g(x(t)) \;=\; (g!)^2\, A(t)\, r(t)^{-2g}\, \left(1 + O(1/g)\right), \quad \textit{as} \quad g \to \infty. \tag{10}$$

Our next main result is the following asymptotic expression for $C_{n,g}$.

▶ **Theorem 2.** *For g/n in a given closed subinterval of $(0, 1/2)$, let $\tau \in (0,1)$ be determined by $\theta(\tau) = g/n$. Then the number $C_{n,g}$ of cubic maps with $2n$ vertices and genus g satisfies*

$$C_{n,g} \;\sim\; (g!)^2 \frac{A(\tau)}{\sqrt{2\pi\, g\, \sigma^2(\tau)}}\, x(\tau)^{-n}\, r(\tau)^{-2g}, \quad \textit{as} \quad g \to \infty. \tag{11}$$

Using (11) and (1) we also obtain the following asymptotic formula for the number of triangular maps (i.e. triangulations) with n vertices and genus g:

$$T_{n,g} \;\sim\; (g!)^2 \frac{A(\tau)\, x(\tau)^2}{\sqrt{2\pi\, g\, \sigma^2(\tau)}}\, x(\tau)^{-n}\, \left(x(\tau) r(\tau)\right)^{-2g}, \quad \text{as} \quad g \to \infty. \tag{12}$$

The rest of the paper is organized as follows. In the next section, we provide proofs of Theorems 1 and 2. In Section 4 we extend Theorem 2 to cover the boundary cases $g/n \to 0$ or $g/n \to 1/2$ (Theorem 3). In Section 5 we compare our asymptotic result on $C_{n,g}$ with a very recent result on the asymptotic number of triangular maps by Budzinski and Louf [6]. We conclude the paper with further discussions on cubic graphs on orientable surfaces in Section 6.

2 Proof of Theorems 1 and 2

Proof of Theorem 1. We begin with the function $F_g(x)$ defined by

$$F_g(x) \;=\; 3x^3 C_g'(x) + 2x^2 C_g(x) \quad (g \ge 0). \tag{13}$$

Rewriting (13) in [5], which is derived from the Goulden-Jackson recursion for cubic maps [14], we obtain the following recursion: for $g \ge 1$,

$$\begin{aligned}&\frac{1-t}{1+2t}F_g(x)+x^2C_g(x)\\&\quad = 36x^4F''_{g-1}(x)+12x^3F'_{g-1}(x)+6x^3\delta_{g,1}+12\sum_{h=1}^{g-1}F_h(x)F_{g-h}(x),\end{aligned} \tag{14}$$

where $\delta_{g,1}$ is equal to 1 if $g=1$ and 0 otherwise.

Furthermore, by definition of the functions $x(t)$ and $r(t)$ in (5)–(7) and with some computation, we obtain

$$\frac{dx}{dt} = \frac{1}{4}(1-t)(1+2t)^{-5/2}, \tag{15}$$

$$\frac{x(t)}{x'(t)} = t+\frac{3t^2}{1-t}, \tag{16}$$

$$\frac{dr}{dt} = -\frac{1}{3}t^{-2}(1-t)^{3/2}, \tag{17}$$

$$\frac{dr}{dx} = -\frac{4}{3}t^{-2}(1-t)^{1/2}(1+2t)^{5/2}, \tag{18}$$

$$\frac{d^2r}{dx^2} = \frac{8}{3}t^{-3}(1-t)^{-3/2}(1+2t)^4(4t^2-5t+4). \tag{19}$$

In terms of the new parameter t, the expression for $C_1(x)$ found in [5] becomes

$$C_1(t) = \frac{t(1+2t)}{4(1-t)^2}. \tag{20}$$

It follows from (5) and (13) that

$$F_1(t) = \frac{t^3(t+5)}{64(1+2t)(1-t)^4}. \tag{21}$$

To derive the asymptotic expression (10), we write

$$C_g(x) = (g!)^2r(t)^{-2g}A_g(t),\ \ A_g(t) = A(t)+a_1(t)g^{-1}+a_2(t)g^{-2}+\cdots,$$

and substitute it into (14). We note

$$\sum_{h=2}^{g-2}\frac{(h!(g-h)!)^2}{(g!)^2} = \sum_{h=2}^{g-2}\left(\binom{g}{h}\right)^{-2} = O\left(g^{-4}\right),$$

$$C'_g(x) = (g!)^2r(t)^{-2g}\left(A'_g(t)-\frac{2gr'(t)A_g(t)}{r(t)}\right)\frac{1}{x'(t)}.$$

Divide both sides of (14) by $(g!)^2$ and expand the resulting expressions in powers of g. Both sides become Laurent series in g with highest power equal to 1. Comparing the coefficients of g and using (13) and (5), we obtain (with the help of computer algebra system *Maple*)

$$r'(t) = -\frac{1}{3}t^{-2}(1-t)^{3/2},$$

which is (17). Observing $\lim_{t\to 1} r(t)=0$ (see (31) in Section 4), we obtain (7).

Next we compare the coefficients of g^0 in Laurent series to obtain

$$\frac{A'(t)}{A(t)} = \frac{11-2t}{4(1-t)(1+2t)}+\frac{(1-t)^{3/2}}{2t^2r(t)}. \tag{22}$$

Integrating both sides, we obtain (9) for some constant K. The approximate value of K is obtained in Section 3. ◀

Proof of Theorem 2. Define functions $u(t)$ and $\mu(t)$ in $t \in (0,1)$ by

$$u(t) := -2\ln r(t), \tag{23}$$

$$\mu(t) := \frac{x(t)}{x'(t)}\frac{du}{dt}. \tag{24}$$

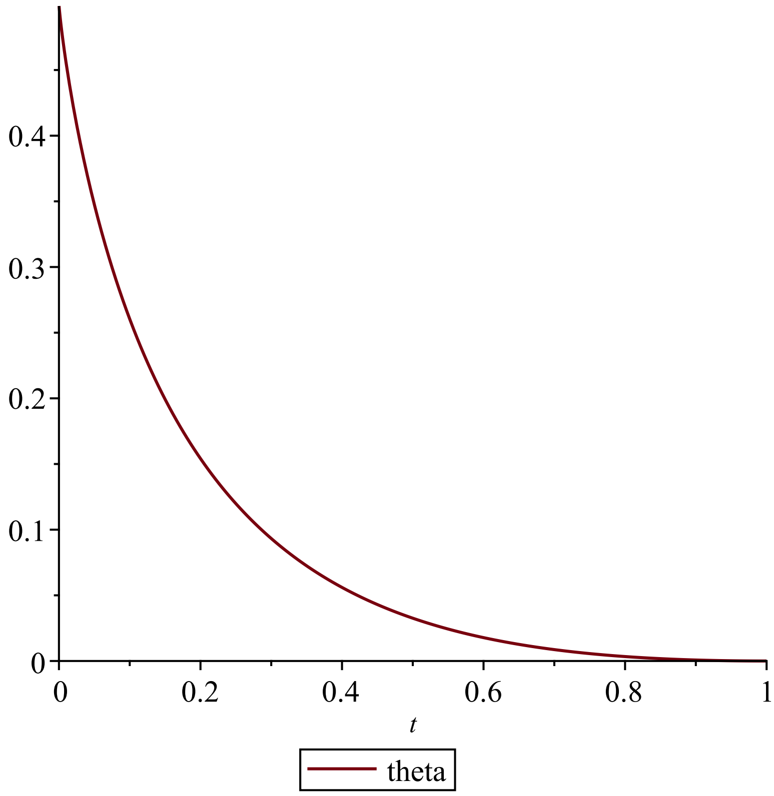

Figure 1 The plot of $\theta(t)$.

With some algebra (and with help of Maple), we find $\theta(t) = 1/\mu(t)$ and $\sigma^2(t) = \frac{x(t)}{x'(t)}\frac{d\mu}{dt}$ are as in (6) and (8), respectively (see Figures 1–2). We note that $\sigma^2(t)$ is positive for $t \in (0,1)$.

In order to apply a generalized version (Theorem 4 in [12]) of the local limit theorem in [2, Theorem 3], we need to verify the technical condition that

$$|r(x)| > r(|x|), \quad \text{for } |x| \in \left(0, 1/(12\sqrt{3})\right) \text{ and } x \neq |x|. \tag{25}$$

We first check (by Maple) that

$$r(t) = \frac{1}{3t} + \frac{1}{2} - \ln 2 - \frac{1}{2}\ln\frac{1}{t} - \frac{1}{8}t - \frac{1}{96}t^2 - \frac{1}{384}t^3 - \frac{1}{1024}t^4 - \cdots,$$

where all the positive powers of t have negative coefficients. Applying the Lagrange inversion formula to (5), we see that $t(x)$ is a power series in x such that $[x^n]t(x)$ are all positive for all $n \geq 1$. Also the radius of convergence of $t(x)$ is $1/(12\sqrt{3}) \doteq 0.048$. This implies that $|t(x)| < t(|x|)$ for all $x \neq |x|$ with $|x| \in (0, 1/(12\sqrt{3}))$, which leads to (25). Figure 3 shows the plots of $|r(\rho e^{i\phi})|$ for $\rho \in \{0.01, 0.02, 0.03, 0.04\}$ and $0 \leq \phi \leq \pi$.

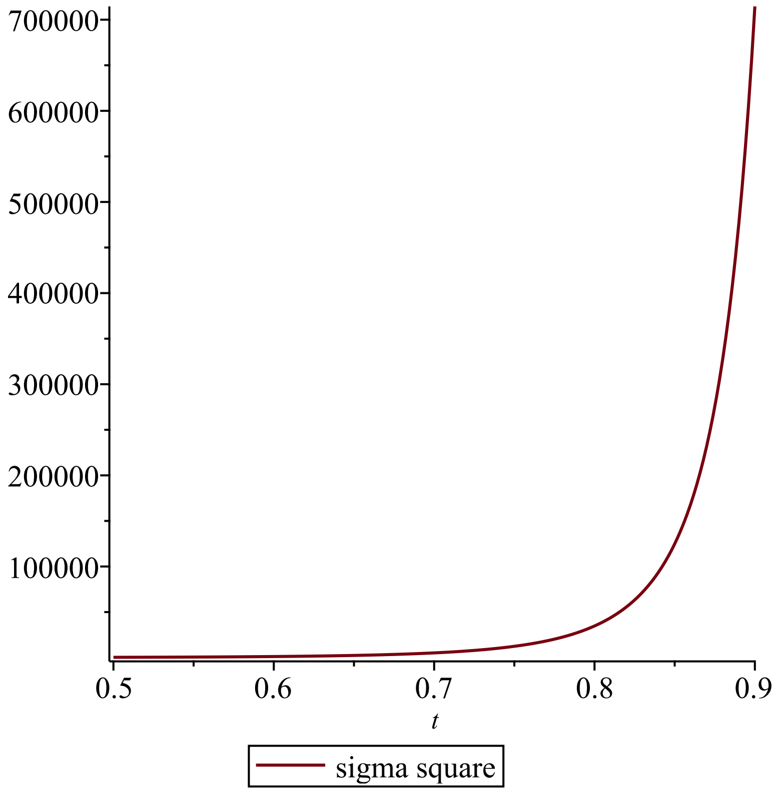

Figure 2 The plot of $\sigma^2(t)$.

Applying [12, Theorem 4] and using (23)–(24), we obtain

$$C_{n,g} \sim (g!)^2 A(\tau) r(\tau)^{-2g} x(\tau)^{-n} \frac{1}{\sqrt{2\pi\, g\, \sigma^2(\tau)}}.$$

This completes the proof of Theorem 2. ◀

3 Estimate the value of K

Our approach in the previous section does not give any information about the constant K that appeared in $A(t)$ – see (9). We may compare the exact values of $C_{n,g}$ and its asymptotic values given by (2) to obtain numerical estimation of K.

Define

$$B_{n,g} := \frac{3n+2}{(g!)^2} C_{n,g} \quad \text{for} \quad n \geq 1, g \geq 0.$$

It follows from the Goulden-Jackson recursion [5, (8)] that

$$\begin{aligned} B_{-1,0} &= 1/2, \\ B_{0,0} &= 2, \\ B_{-1,g} &= B_{0,g} = 0 \quad \text{for} \quad g \geq 1, \end{aligned}$$

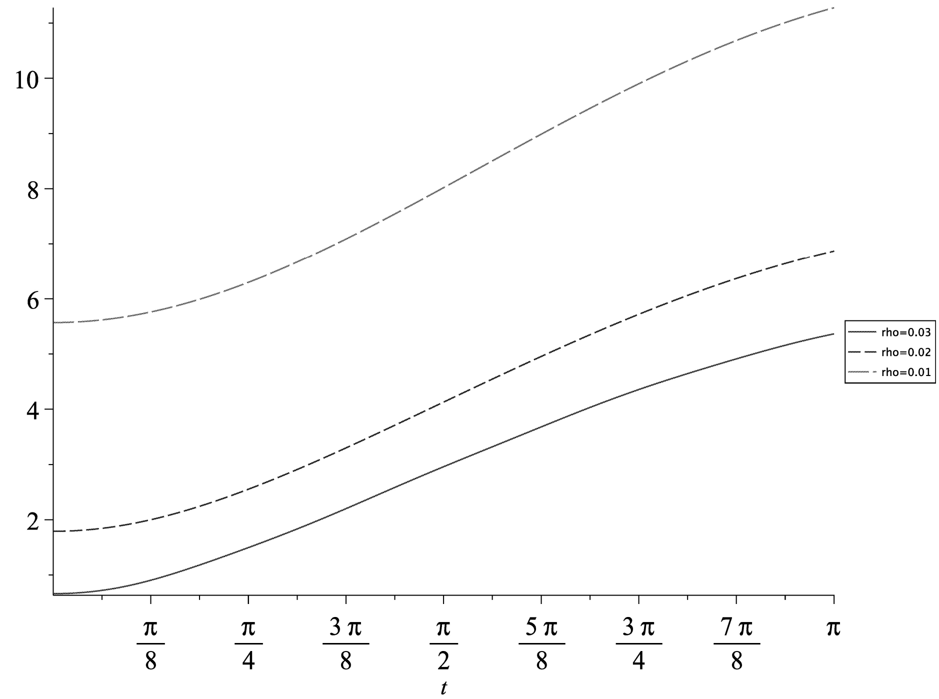

Figure 3 The plots of $|r(\rho e^{i\phi})|$.

and for $n \geq 1, g \geq 0$,

$$B_{n,g} = \frac{4(3n+2)}{n+1}\left(\frac{n(3n-2)}{g^2}B_{n-2,g-1} + \sum_{i=-1}^{n-1}\sum_{h=0}^{g}\frac{1}{\binom{g}{h}^2}B_{i,h}B_{n-2-i,g-h}\right), \tag{26}$$

where $B_{n-2,g-1}/g^2$ is understood to be 0 when $g = 0$.

Using (9) and (11) we obtain

$$\ln K \doteq \ln B_{n,g} - \frac{1}{2}\ln g + g\left(\frac{\ln x}{\theta} + 2\ln r\right) + \frac{1}{2}\ln\left(2\pi\sigma^2\right) - \ln\frac{3}{\theta} - \left(\ln\frac{27}{8} - \frac{1}{2}\ln(1+2t) + \frac{3}{2}\ln\frac{t}{2(1-t)\theta}\right).$$

We used $\theta = 1/3$ and calculated $B_{3g,g}$ for $1 \leq g \leq 150$ using (26). We then obtain

$$t \doteq 0.0569135164, x \doteq 0.0121039967, r \doteq 4.223432731, \sigma^2 \doteq 1.212044822, K \doteq 1.2 \times 10^{-6}.$$

4 Extend to the boundary

In this section we extend Theorem 2 to cover the ranges of g satisfying $g/n \to 0$ or $g/n \to 1/2$. More specifically, we shall apply the saddle-point method to prove

▶ **Theorem 3.** *Assume the same notation as in Theorem 2. Then* (11) *and* (12) *hold when*

$$g \to \infty \quad \text{and} \quad \frac{n}{2} - g \to \infty \quad \text{as } n \to \infty. \tag{27}$$

Proof Sketch. To study the asymptotic behaviours of $C_{n,g}$ when $\theta = g/n$ is near 0 or 1/2, we need to find the asymptotic expansions of relevant functions as $t \to 0$ or $t \to 1$. With the help of *Maple* and using (5)–(9), we obtain the following asymptotic expansions.

$$x(t) = \begin{cases} \frac{t}{4} - \frac{3t^2}{4} + O\left(t^3\right), & t \to 0, \\ \frac{1}{12\sqrt{3}}\left(1 - \frac{1}{6}(1-t)^2 - \frac{5}{27}(1-t)^3 + O\left((1-t)^4\right)\right), & t \to 1, \end{cases} \tag{28}$$

$$\frac{x(t)}{x'(t)} = \begin{cases} t + 3t^2 \sum_{k\geq 0} t^k, & t \to 0, \\ 3(1-t)^{-1} - 5 + 2(1-t), & t \to 1, \end{cases} \tag{29}$$

$$\theta(t) = \begin{cases} \frac{1}{2} + \frac{3t}{4}\ln\frac{t}{4} + O\left(t^2 \ln t\right), & t \to 0, \\ \frac{1}{15}(1-t)^2 + \frac{23}{315}(1-t)^3 + O\left((1-t)^4\right), & t \to 1, \end{cases} \tag{30}$$

$$r(t) = \begin{cases} \frac{1}{3t} + \frac{1}{2}\ln\frac{et}{4} + O(t), & t \to 0, \\ \frac{2}{15}(1-t)^{5/2} + \frac{4}{21}(1-t)^{7/2} + O\left((1-t)^{9/2}\right), & t \to 1. \end{cases} \tag{31}$$

$$\mu(t) = \begin{cases} 2 - 3t\ln t + (6\ln 2)t + O\left((t\ln t)^2\right), & t \to 0, \\ 15(1-t)^{-2} + O\left((1-t)^{-1}\right), & t \to 1, \end{cases} \tag{32}$$

$$\sigma^2(t) = \begin{cases} -3t\ln t + O(t), & t \to 0, \\ 90(1-t)^{-4} + O\left((1-t)^{-3}\right), & t \to 1, \end{cases} \tag{33}$$

$$M_3(t) := \frac{x(t)}{x'(t)}\frac{d\sigma^2}{dt} = \begin{cases} -3t\ln t + O(t), & t \to 0, \\ 1080(1-t)^{-6} + O\left((1-t)^{-5}\right), & t \to 1, \end{cases} \tag{34}$$

$$A(t) = \begin{cases} \frac{27K}{8}t^{3/2} + O\left(t^{5/2}\ln t\right), & t \to 0, \\ \frac{405\sqrt{10}K}{32}(1-t)^{-9/2} + O\left((1-t)^{-7/2}\right), & t \to 1. \end{cases} \tag{35}$$

A more careful analysis of (10) gives

$$C_g(x) \;=\; (g!)^2\, A(t)\, r(t)^{-2g}\, (1 + O\,(1/g))\,,$$

where the O-term is uniform for $0 < t < 1$. In fact, we have (with the help of Maple)

$$A_g(t) = A(t)\left(1 - \frac{3}{8}\left(2 + \frac{20t^2 - 42t + 31}{1+2t}\frac{t\,r(t)}{(1-t)^{5/2}}\right)g^{-1} + O(g^{-2})\right). \tag{36}$$

Using (31), we see that the coefficient of g^{-1} in (36) is bounded for $t \in (0,1)$.

The Cauchy integration formula and the standard saddle-point method give

$$\begin{aligned}
[x^n]C_g(x) &= \frac{1}{2\pi i}\oint_{|x|=x(\tau)} C_g(x)x^{-n-1}dx \\
&\sim \frac{(g!)^2}{2\pi}x(\tau)^{-n}\int_{|\phi|\leq\pi} A(\tau e^{i\phi})\exp\left(gu(\tau e^{i\phi})\right)e^{-in\phi}d\phi \\
&\sim \frac{(g!)^2}{2\pi}A(\tau)x(\tau)^{-n}r(\tau)^{-2g}\int_{|\phi|\leq\delta}\exp\left(-\frac{g\sigma^2(\tau)\phi^2}{2} + O\left(gM_3(\tau)\delta^3\right)\right)d\phi,
\end{aligned}$$

where τ is determined by the saddle-point equation $\theta(\tau) = g/n$, $M_3(\tau)$ is given in (34), and δ satisfies

$$g\sigma^2(\tau)\delta^2 \to \infty \quad \text{and} \quad gM_3(\tau)\delta^3 \to 0.$$

It follows from (33) and (34) that this condition is satisfied, provided that

$$gt\ln(1/t) \to \infty \quad \text{as} \quad t \to 0. \tag{37}$$

Using (30), we see that (37) is equivalent to

$$g\left(\frac{1}{2} - \frac{g}{n}\right) \to \infty \quad \text{as} \quad \frac{g}{n} \to \frac{1}{2}, \quad \textit{i.e.} \quad \frac{n}{2} - g \to \infty \quad \text{as} \quad \frac{g}{n} \to \frac{1}{2}.$$

This completes the proof of Theorem 3. ◀

When the order of g/n or $n-2g$ is known, the asymptotic expression of $C_{n,g}$ can be simplified using the asymptotic expansions (29)–(36). For example, we have the following corollary to Theorem 3.

▶ **Corollary 4.** *Let $\theta = g/n$. Suppose $g \to \infty$ and $g = o\left(n^{1/2}\right)$. Then*

$$C_{n,g} \sim \frac{9K}{32\,(15)^{1/4}\sqrt{2\pi g}}\theta^{-5/4}\,(g!)^2\left(12\sqrt{3}\right)^n \exp\left(\left(\frac{5}{2}\ln\frac{e}{15\theta}+2\ln\frac{15}{2}-\frac{5}{63}(15\theta)^{1/2}\right)g\right).$$

Proof. When $g = o(n^{1/2})$, we have the following expansions

$$\begin{aligned}
1-t &= (15\theta)^{1/2}\left(1-\frac{23}{42}(15\theta)^{1/2}+O(\theta)\right),\\
A &\sim \frac{405K\sqrt{10}}{32}(15\theta)^{-9//4},\\
\sigma &\sim 3\sqrt{10}(15\theta)^{-1},\\
\ln x &= \ln\frac{1}{12\sqrt{3}}-\frac{5}{2}\theta-\frac{5}{27}(15\theta)^{3/2}+O\left(\theta^2\right),\\
\ln r &= \ln 2+\frac{1}{4}\ln 15+\frac{5}{4}\ln\theta+\frac{10}{7}(15\theta)^{1/2}+O(\theta),\\
r^{-2g}x^{-n} &\sim (12\sqrt{3})^n\exp\left(g\left(\frac{5}{2}-\ln 4-\frac{1}{2}\ln 15-\frac{5}{2}\ln\theta-\frac{5}{63}(15\theta)^{1/2}\right)\right).
\end{aligned}$$

Now the result follows from Theorem 3. ◀

The following result from [6] is an immediate consequence of Theorem 2.

▶ **Corollary 5.** *Let $g, n \to \infty$ such that $g/n \to \theta_0 \in (0, 1/2)$. Let t_0 be determined by $\theta(t_0) = \theta_0$ and $x_0 = x(t_0)$, where $x(t)$ and $\theta(t)$ are defined by (6) and (5). Then we have*

$$\frac{C_{n+1,g}}{C_{n,g}} \to \frac{1}{x_0}, \quad \text{as} \quad n \to \infty.$$

Proof. Let t_1 be determined by $\theta(t_1) = g/(n+1)$. Since

$$\frac{g}{n+1} = \theta_0 - \frac{\theta_0}{n} + O\left(\frac{\theta_0}{n^2}\right),$$

and the function $\theta(t)$ is differentiable and has nonzero derivative in $(0, 1)$, we have

$$t_1 = t_0 + O\left(\frac{1}{n}\right).$$

Hence

$$x(t_1) \to x(t_0),\ r(t_1) \to r(t_0),\ A(t_1) \to A(t_0),\ \sigma^2(t_1) \to \sigma^2(t_0) \quad \text{as} \quad n \to \infty.$$

Writing $f(t) := \ln x(t) + 2\theta_0 \ln r(t)$ and applying Theorem 2, we obtain

$$\begin{aligned}
\frac{C_{n+1,g}}{C_{n,g}} &\sim \frac{1}{x(t_0)}\left(\frac{x(t_1)}{x(t_0)}\right)^{-n}\left(\frac{r(t_1)}{r(t_0)}\right)^{-2g}\\
&= \frac{1}{x(t_0)}\exp\left(-n\left(f(t_1)-f(t_0)\right)\right)\\
&= \frac{1}{x(t_0)}\exp\left(-n\left(f'(t_0)(t_1-t_0)+O\left((t_1-t_0)^2\right)\right)\right).
\end{aligned}$$

Using (23) and (24) and noting $\theta_0 = 1/\mu(t_0)$, we obtain

$$f'(t_0) = \frac{x'(t_0)}{x(t_0)} + 2\theta_0 \frac{r'(t_0)}{r(t_0)} = 0.$$

Thus

$$\frac{C_{n+1,g}}{C_{n,g}} \sim \frac{1}{x(t_0)} \exp\left(-O\left(n/n^2\right)\right) \to \frac{1}{x_0},$$

as desired. ◀

5 Cross-check with a result on triangulations in [6]

In [6] Budzinski and Louf resolved a conjecture of Benjamini and Curien on the local limits of uniform random triangulations whose genus is proportional to the number of faces. As a consequence, they derived an asymptotic formula for the number of triangulations up to sub-exponential factors.

Using notations in [6], let $\tau(n, g)$ denote the number of triangulations (i.e. triangular maps) with $2n$ faces and genus g, which of course is equal to the number $C_{n,g}$ to cubic maps (as dual) with $2n$ vertices and genus g. For any $\lambda \in (0, 1/(12\sqrt{3})]$ let $h \in (0, 1/4]$ be such that

$$\lambda = \frac{h}{(1+8h)^{3/2}} \quad \text{and} \quad \psi(\lambda) = \frac{h \ln\left(1+\sqrt{1-4h})/(1-\sqrt{1-4h}\right)}{(1+8h)\sqrt{1-4h}}.$$

For any $\vartheta \in [0, 1/2)$ let $\lambda = \lambda(\vartheta)$ be the unique solution of the equation

$$\psi(\lambda) = \frac{1-2\vartheta}{6}.$$

In [6, Theorem 3] it was shown that for $g = g(n)$ satisfying $0 \le g \le \frac{n+1}{2}$ and $g/n \to \vartheta \in [0, 1/2]$, we have

$$\tau(n, g) \ = \ n^{2g} \exp(f(\vartheta)\, n + o(n)), \quad \text{as} \quad n \to \infty, \tag{38}$$

where $f(0) = \log(12\sqrt{3})$, $f(1/2) = \log(6/e)$, and

$$f(\vartheta) \ = \ 2\vartheta \ln(12\vartheta/e) - (1-2\vartheta) \int_{2\vartheta}^{1} \ln \lambda(\vartheta/z) dz, \quad \text{for} \quad \vartheta \in (0, 1/2),$$

in which we have corrected the factor $-(1-2\vartheta)$ in front of the integral – see (3) in [6, Theorem 3] for comparison.

In order to compare (38) with our result (11), we note the following relations between parameters:

$$t = 4h, \quad x = \lambda, \quad \mu = \frac{1}{\vartheta}.$$

Using Stirling's formula (up to the sub-exponential factor), we may rewrite our asymptotic expression of $C_{n,g}$ in (11) as

$$C_{n,g} \ \approx \ n^{2g} \exp(q(t)\, n), \quad \text{as} \quad n \to \infty, \tag{39}$$

where

$$q(t) \ = \ 2(-\ln r + \ln \theta - 1)\theta - \ln x. \tag{40}$$

We note that, as $t \to 0$, $\theta \to 1/2$ and consequently

$$q(t) \;\to\; -\ln(rx) - \ln(2e) \;\to\; \ln(6/e) \;=\; f(1/2).$$

As $t \to 1$, we have $\theta \to 0$ and

$$q(t) \;\to\; 2\theta \ln(\theta/r) - \ln x \;\to\; \ln 12\sqrt{3} \;=\; f(0).$$

These two values match with those in (38).

6 Discussions: cubic graphs on orientable surfaces

Graphs that are closely related to cubic maps on Σ_g are cubic graphs with genus at most g, which play a crucial role in the study of phase transitions in sparse random graphs on orientable surfaces, as it was shown in [8, 15]. Let $\tilde{H}_{n,g}$ denote the number of vertex-labeled cubic graphs with $2n$ vertices and genus at most g and let $H_{n,g} = \tilde{H}_{n,g}/(2n)!$. In [8, 9], it was shown that if g is constant, then

$$H_{n,g} \;\sim\; c_g\, n^{5(g-1)/2-1}\gamma^n,$$

where γ does not depend on g and is the same constant as planar case (i.e. when $g = 0$), and if $g \le \frac{n+1}{2}$, then

$$a_g\, n^{2g} \;\le\; H_{n,g} \;\le\; b_g\, g^{-4g}\, n^{6g}. \tag{41}$$

Note that if $g > \frac{n+1}{2}$, then $H_{n,g}$ is equal to the total number of cubic graphs with $2n$ vertices (without restriction on the genus). Therefore, we have

$$H_{n,g} \;\sim\; e^{-2}\,\frac{(6n-1)!!}{(3!)^{2n}} \;=\; e^{-2}\,\frac{(6n)!}{(3n)!\,2^{3n}\,(3!)^{2n}} \;\sim\; e^{-2}\left(\frac{6}{e^3}\right)^n n^{3n}. \tag{42}$$

So far, an asymptotic expression for $H_{n,g}$ when $g/n \in (0, 1/2]$ is not known.

▶ **Problem 1.** *Derive an asymptotic expression for $H_{n,g}$ when $1 \ll g \le \frac{n+1}{2}$.*

As it turned out, it is quite difficult to resolve Problem 1. Let us first compare asymptotic behaviors of $H_{n,g}$ and $C_{n,g}$, particularly when $g/n \to 1/2$. If the asymptotic formula (11) of $C_{n,g}$ *would* hold also for $g/n \to 1/2$, then

$$C_{n,g} \;\approx\; n^n, \quad \textit{as} \quad g/n \to 1/2. \tag{43}$$

The upper bound in (41) indicates that the super-exponential factor of $H_{n,g}$ could be

$$H_{n,g} \;\approx\; n^n, \quad \text{as} \quad g/n \to 1/2, \tag{44}$$

which matches with (43). Note however that (42) suggests that the super-exponential factor of $H_{n,g}$ might be

$$H_{n,g} \;\approx\; n^{3n}, \quad \text{as} \quad g/n \to 1/2, \tag{45}$$

which is substantially larger than (43).

It would be interesting to check whether or not the asymptotic formula of $C_{n,g}$ in Theorem 2 holds even for $g/n \to 1/2$.

▶ **Problem 2.** *Determine asymptotic behavior of $C_{n,g}$ when $g/n \to 1/2$.*

Another natural, but challenging task in view of (44) and (45) is the following.

▶ **Problem 3.** *Does there exist a threshold function $t^* = t^*(n) = o(n)$ such that*

$$H_{n,g} \;\approx\; \begin{cases} n^n, & \text{as} \quad g - n/2 = o(t^*), \\ n^{h(c)\, n}, & \text{as} \quad g - n/2 = c\, t^* \quad (\text{for} \quad c \in \mathbb{R}), \\ n^{3n}, & \text{as} \quad g - n/2 = \omega(t^*), \end{cases}$$

for some function $h : \mathbb{R} \to [1, 3]$ satisfying $h(c) \to 1$ as $c \to -\infty$ and $h(c) \to 3$ as $c \to \infty$?

As very recent results on sparse random graphs with large genus [8] revealed, the most interesting unknown case is when the genus is linear in the number of vertices.

▶ **Problem 4.** *Derive an asymptotic expression for $H_{n,g}$ when $g/n \in (0, 1/2]$.*

To this end, we may apply the following steps (analogous ideas were successfully utilized in [9] when g is constant).

(S1) We first derive asymptotic formula for 2-connected cubic maps (equivalently, loopless triangular maps) of genus $g = \theta n$. This will be done as follows.
- Show that triangular maps with a non-contractible loop are negligible by cutting through such a loop and bounding the number of such maps by triangular maps of genus $g - 1$.
- For contractible loops, we can apply the usual composition technique to derive equations of generating functions relating loopless triangular maps and all triangular maps.

(S2) Similarly, we derive formulas for 3-connected cubic maps (equivalently, triangular maps without loops or multiple edges).

(S3) In order to go from 3-connected cubic *maps* on Σ_g to 3-connected cubic *graphs* on Σ_g, we apply Robertson-Vitray uniqueness embedding result or Thomassen's LEW result (see e.g. [17]). We need to show that almost all such cubic maps have representativity larger than $2g+3$ (equivalently, all non-contractible cycles have length greater than $2g+3$).

(S4) Finally, in order to go from 3-connected cubic graphs to cubic graphs with lower connectivity we apply standard connectivity-decomposition arguments.

Note that (S3) can be quite challenging since the genus g is linear in n, and we only have g^2 to play with the error term.

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Diffusion Limits in the Online Subsequence Selection Problems

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Abstract

In the stochastic sequential optimisation problems it is of interest to study features of strategies more delicate than just their performance measure. In this talk we focus on variations of the online monotone subsequence and bin packing problems, where it is possible to give a fairly explicit asymptotic description of the selection processes under strategies that are sufficiently close to optimality. We show that the transversal fluctuations of the shape and the length of selected subsequence approach Gaussian functional limits that are very different from their counterparts in the offline problem, where the full set of data can be used in selection algorithms.

2012 ACM Subject Classification Mathematics of computing → Markov processes

Keywords and phrases sequential optimisation, longest increasing subsequence, bin packing, fluctuations in the selection process, functional limit

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.14

Related Version `https://arxiv.org/abs/2001.02249`

1 Introduction

In many stochastic optimisation problems units of the data become available in real time, whereas admissible decision strategies involve a series of irrevocable choices. The analysis of such problems is largely focused on finding optimal or near-optimal strategies to maximise a given performance criterion subject to constraints. Much less attention has been devoted to the structure of decison processes as a whole, in all intermediate states.

In this paper we mainly focus on the online monotone subsequence problem of Samuels and Steele [18]. Suppose i.i.d. marks drawn from the uniform distribution on $[0, 1]$ are observed, one by one, at times of an independent homogeneous Poisson process of intensity ν on $[0, 1]$. Each mark can be selected or rejected. The sequence of selected marks must increase. The task is to maximise the expected length of selected increasing subsequence using an online strategy. The online constraint requires that each decision becomes immediately irrevocable as the mark is observed, and must be based exclusively on the information accumulated previously without foresight of the future.

The optimal online strategy is defined recursively in terms of a variable acceptance window, which limits the difference between the next and previous selections. The strategy and its value can be found, in principle, by solving a dynamic programming equation, see [4, 6, 11] for properties of the solution and approximations. We are interested in the time evolution of increasing subsequences under online strategies that are within $O(1)$ gap from the optimum for large ν.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 14; pp. 14:1–14:15
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

Let $L_\nu(t)$ and $X_\nu(t)$, respectively, denote the length and the last element of the increasing subsequence selected by time $t \in [0,1]$ under the optimal strategy. The interest to date focused on the total length $L_\nu(1)$. Samuels and Steele derived the principal asymptotics $\mathbb{E}L_\nu(1) \sim \sqrt{2\nu}$, which was later found to be an upper bound with the optimality gap of order $\log \nu$ [6]. See [1, 2, 4, 6, 10] for refinements and generalisations. In a recent paper [11] we combined asymptotic analysis of the dynamic programming equation with a renewal approximation to the range of the process $Z_\nu(t) := \sqrt{\nu(1-t)(1-X_\nu(t))}$ to derive expansions for the mean

$$\mathbb{E}L_\nu(1) \sim \sqrt{2\nu} - \frac{1}{12}\log \nu + c_0^*, \quad \nu \to \infty, \tag{1}$$

and the variance

$$\operatorname{Var} L_\nu(1) \sim \frac{1}{3}\sqrt{2\nu} - \frac{1}{72}\log \nu + c_1^*, \quad \nu \to \infty, \tag{2}$$

where c_0^* and c_1^* are unknown constants. A central limit theorem for $L_\nu(1)$ was proved in [7] by analysis of a related martingale, and further extended in [11] to a larger class of asymptotically optimal strategies by the mentioned renewal theory approach.

The offline counterpart of the selection problem is the Ulam-Hammersley problem on the longest increasing subsequence of the Poisson scatter in the square $[0,1]^2$. Here, the well known principal asymptotics of the expected maximum length, $2\sqrt{\nu}$, is similar, but the second term of its asymptotic expansion and the principal term of the standard deviation are both of the order $\nu^{1/6}$. The limit law for the offline maximum length is the Tracy-Widom distribution from the random matrix theory. For survey and history see [17].

In the offline problem, some work has been done on the size of transversal fluctuations about the diagonal $x = t$ in $[0,1]^2$. Johansson [12] proved a measure concentration result asserting that, with probability approaching 1, every longest increasing subsequence (which is not unique) lies in a diagonal strip of width of the order $\nu^{-1/6+\epsilon}$. Duvergne, Nica and Virág [8] recently proved the existence and gave some description of the functional limit, which is not Gaussian. But for smaller exponent $-1/2 < \alpha < -1/6$, Joseph and Peled [15] showed that if the increasing sequence is restricted to lie within the strip of width $\nu^{-\alpha}$, the expected maximum length remains to be asymptotic to $2\sqrt{\nu}$, while the limit distribution of the length switches to normal.

To extend the parallels and gain further insight into the optimal selection it is of considerable interest to examine fluctuations of the processes L_ν and X_ν as a whole. On this path, one is lead to study the following scaled and centred versions of the running maximum and length processes:

$$\widetilde{X}_\nu(t) := \nu^{1/4}(X_\nu(t) - t), \qquad \widetilde{L}_\nu(t) = \nu^{1/4}\left(\frac{L_\nu(t)}{\sqrt{2\nu}} - t\right), \quad t \in [0,1]. \tag{3}$$

To compare, in the offline problem by similar centring the critical transversal and longitudinal scaling factors appear to be $\nu^{1/6}$ and $\nu^{1/3}$, respectively. Our central result (Theorem 4) is a functional limit theorem which entails that the process $(\widetilde{X}_\nu, \widetilde{L}_\nu)$ converges weakly to a simple two-dimensional Gaussian diffusion. In particular, $\widetilde{X}_\nu$ approaches a Brownian bridge. The limit of $\widetilde{L}_\nu$ is a non-Markovian process with the covariance function

$$(s,t) \mapsto \frac{2s(2-t) - (2-s-t)\log(1-s)}{6\sqrt{2}}, \quad 0 \le s \le t \le 1,$$

which corresponds to a correlated sum of a Brownian motion and a Brownian bridge.

The question about functional limits for L_ν and X_ν has been initiated by Bruss and Delbaen [7]. They employed the Doob-Meyer decomposition to compensate the processes, and in an analytic tour de force showed that the scaled martingales jointly converge to a correlated Brownian motion in two dimensions. However, the compensation keeps out of sight a drift component absorbing much of the fluctuations immanent to the selection process, let alone that the compensators themselves are nonlinear integral transforms of X_ν. Looking at the generator of (3) we shall recognise the limit process without difficulty, showing that this is a Gaussian diffusion driven by the same Brownian motion as in [7]. But in order to justify the weak convergence in the Skorokhod space on the closed interval $[0, 1]$ we will need to circumvent a difficulty caused by pole singularities of the control function and the drift coefficient at the right endpoint.

A mathematically equivalent problem appears if the monotonicity condition is replaced by the constraint that the sum of of selected marks cannot exceed 1. A more general form of the latter "online bin-packing" problem has also been studied in the literature [9, 16], under the assumption that (positive) marks are sampled from some distribution with regular behaviour near 0. In the last section we sketch functional limit results for this bin-packing problem.

2 Selection strategies

It will be convenient to extend slightly the underlying framework by considering a homogeneous Poisson random measure Π with intensity ν in the halfplane $\mathbb{R}_+ \times \mathbb{R}$, along with the filtration induced by restricting Π to $[0, t] \times \mathbb{R}$ for $t \geq 0$. We interpret the generic atom (t, x) of Π as random mark x observed at time t. A sequence $(t_1, x_1), \dots, (t_\ell, x_\ell)$ of atoms is said to be increasing if it is a chain in two dimensions, i.e. $t_1 < \cdots < t_\ell,\ x_1 < \cdots < x_\ell$.

For a given bounded measurable *control* function $\psi : [0, 1] \times \mathbb{R} \to \mathbb{R}_+$, an online strategy selecting such increasing sequence is defined by the following intuitive rule. Let x be the last mark selected before time t, or some given x_0 if no selection has been made. Given the next mark x' is observed at time t, this mark is selected if and only if $x < x' \leq x + \psi(t, x)$. One can think of more general online strategies, with the acceptance window shaped differently from an interval or possibly depending on the history in a more complex way. Yet the considered class is sufficient for the sake of optimisation and can be further reduced to controls of a special type.

For a given control ψ, define $X(t)$ and $L(t)$ to be, respectively, the last mark selected and the number of marks selected within the time interval $[0, t]$. The process $X = (X(t),\ t \in [0, 1])$, which we call the *running maximum*, is a time-inhomogeneous Markov process, jumping from the generic state x at rate $\psi(t, x)$ to another state uniformly distributed on $[x, x + \psi(t, x)]$. The *length process* $L = (L(t),\ t \in [0, 1])$ just counts the jumps of X, hence the bivariate process (X, L) is also Markovian. Moreover, the conditional distribution of $((X(t), L(t)),\ t \geq s)$ depends on the pre-s history only through $X(s)$.

Intuitively, the bigger ψ the faster X and L increase. To enable comparisons of selection processes with different controls it is very convenient to couple them by means of an additive representation through another Poisson random measure Π^*, thought of as a reserve of positive increments. The underlying properties of the planar Poisson process are translation invariance and spatial independence: Π restricted to the shifted quadrant $(t, x) + \mathbb{R}_+^2$ is independent of $\Pi_{|[0,t] \times \mathbb{R}}$ and has the same distribution as the translation of $\Pi_{|\mathbb{R}_+^2}$ by vector (t, x). So, letting Π^* to be a distributional copy of Π, a solution to the system of stochastic differential equations

$$\mathrm{d}X(t) = \int_0^{\psi(t,X(t))} x\,\Pi^*(\mathrm{d}t\mathrm{d}x), \quad \mathrm{d}L(t) = \int_0^{\psi(t,X(t))} \Pi^*(\mathrm{d}t\mathrm{d}x) \tag{4}$$

with initial values $X(0) = x_0$ and $L(0) = 0$ will have the same distribution as (X, L).

▶ **Lemma 1.** *For $i = 1, 2$ let X_i be selection processes driven by controls ψ_i. By coupling via* (4)*, each time a process with smaller acceptance window jumps, the other process also has a jump of the same size.*

Conditionally on $(X(s), L(s)) = (x, \ell)$, the process $(X(s + \cdot) - x, L(s + \cdot) - \ell))$ has the same distribution as $(X^{(s,x)}, L^{(s,x)})$, which similarly to (4) is given by

$$dX^{(s,x)}(u) = \int_0^{\psi(s+u,x+X^{(s,x)}(u))} y\Pi^*(\mathrm{d}u\mathrm{d}y), \quad \mathrm{d}L^{(s,x)}(u) = \int_0^{\psi(s+u,x+X^{(s,x)}(u))} \Pi^*(\mathrm{d}u\mathrm{d}y).$$

Averaging, we obtain formulas for the predictable *compensators* of X and L

$$C_X(t) := \frac{\nu}{2}\int_0^t \psi^2(s, X(s))\mathrm{d}s, \quad C_L(t) := \nu \int_0^t \psi(s, X(s))\mathrm{d}s, \tag{5}$$

so $X - C_X, L - C_L$ are zero-mean martingales.

With every control we may further relate a zero-mean martingale

$$M(t) := L(t) + \mathbb{E}\{L(1) - L(t)|X(t)\} - \mathbb{E}L(1) \tag{6}$$

with terminal value $L(1) - \mathbb{E}L(1)$. If ψ does not depend on x, L has independent increments and $M(t) = L(t) - \mathbb{E}L(t)$.

The selected increasing chain fits in the unit square if $X(1) \le 1$, which translates in terms of the control function as the condition of *feasibility*:

$$0 < \psi(t, x) \le 1 - x \quad \text{for} \quad (t, x) \in [0, 1]^2.$$

In the sequel, if not stated otherwise we set $x_0 = 0$ and only consider feasible controls.

2.1 Principal convergence of the moments

Let

$$p(t) := \mathbb{E}X(t) = \mathbb{E}C_X(t), \quad q(t) := \frac{\mathbb{E}L(t)}{\sqrt{2\nu}} = \frac{\mathbb{E}C_L(t)}{\sqrt{2\nu}}.$$

Some general relations between the moments follow straight from formulas for the compensators (5). For shorthand, write $\psi = \psi(X(s), s)$. We have

$$0 \le \mathbb{E}\int_0^t \left(1 \pm \sqrt{\nu/2}\,\psi\right)^2 \mathrm{d}s = t \pm 2q(t) + p(t),$$

where the right-hand side in increasing in t. It follows,

$$p(t) - t \ge 2\,(q(t) - t). \tag{7}$$

Using the Cauchy-Schwarz inequality

$$(p(t) - t)^2 = \left(\mathbb{E}\int_0^t \left(1 - \frac{\nu}{2}\psi^2\right)\mathrm{d}s\right)^2 \le (t + 2q(t) + p(t))(t - 2q(t) + p(t)). \tag{8}$$

Similarly

$$(q(t)-t)^2 = \left(\mathbb{E}\int_0^t 1\cdot\left(1-\sqrt{\nu/2}\,\psi\right)\mathrm{d}s\right)^2 \le t\,(t-2q(t)+p(t)) \tag{9}$$

The above relations did not use the feasibility constraint. For feasible control we have $p(1) < 1$, hence from (7) also $q(1) < 1$. Since all factors in the right-hand sides of (8), (9) are increasing, replacing them by their maximal values at $t = 1$ we obtain

$$(p(t)-t)^2 < 8(1-q(1)), \quad (q(t)-t)^2 < 2(1-q(1)). \tag{10}$$

We say that a strategy $\psi = \psi_\nu$ is *asymptotically optimal in the principal term* if $q(1) \to 1$, as $\nu \to \infty$, i.e. $\mathbb{E}L_\nu(1) \sim \sqrt{2\nu}$; in that case (10) imply the uniform convergence of the moments

$$\sup_{t\in[0,1]} |p(t)-t| \to 0, \ \sup_{t\in[0,1]} |q(t)-t| \to 0.$$

It follows from (1) that under the optimal strategy

$$1-q(1) \sim \frac{\log\nu}{12\sqrt{2\nu}}, \quad \nu\to\infty. \tag{11}$$

This relation can be called a *two-term asymptotic optimality.* Whenever this holds, the general bounds (10) imply that both $\sup_{t\in[0,1]}|p(t)-t|$ and $\sup_{t\in[0,1]}|q(t)-t|$ can be estimated as $O(\sqrt{\log\nu}/\nu^{1/4})$.

2.2 The stationary strategy

We call the strategy with control $\psi(t,x) = \sqrt{2/\nu}$ *stationary.* Although not feasible, the stationary strategy is an important benchmark. Clearly, L is a Poisson counting process with intensity $\mathbb{E}L(1) = \sqrt{2\nu}$. Taking general constant control $\psi(t,x) = \sqrt{c/\nu}$ with some $c > 0$ will yield a strategy outputting the mean length $\sqrt{\{c \wedge (2/c)\}\nu}$, which is maximal for $c = 2$. In fact, a much stronger optimality property holds: the stationary strategy achieves the maximum expected length over the class of strategies that satisfy the *mean-value* constraint $\mathbb{E}X(1) \le 1$, see [1, 4, 10, 11] for proof and generalisations. This gives the well-known upper bound mentioned in the Introduction, because each feasible strategy meets the mean-value constraint.

It is seen from (4) that X is a compound Poisson process

$$X(t) = \sqrt{\frac{2}{\nu}}\ \sum_{i=0}^{L(t)} U_i\,,$$

where $U_1, U_2, \ldots$ are independent of L, uniformly distributed on $[0,1]$. Straightforward calculation of moments using Wald's identities yields

$$\mathbb{E}X(t) = t, \quad \mathrm{Var}X(t) = \frac{2^{3/2}t}{3\sqrt{\nu}}, \quad \mathrm{Cov}(X(t), L(t)) = t.$$

Since (X, L) has independent increments, a functional limit in the Skorohod topology on $D[0,1]$ follows easily from the multidimensional invariance principle:

$$(\widetilde{X}, \widetilde{L}) \Rightarrow (W_1, W_2), \quad \text{as } \nu\to\infty,$$

where $\Rightarrow$ denotes weak convergence, and the limit process $\boldsymbol{W} := (W_1, W_2)$ is a two-dimensional Brownian motion with zero drift and covariance matrix

$$\mathbb{E}\{\boldsymbol{W}(t)^T\boldsymbol{W}(t)\} = t\,\boldsymbol{\Sigma}, \quad \text{where} \quad \boldsymbol{\Sigma} := \begin{pmatrix} \frac{2\sqrt{2}}{3} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{12}$$

So, marginally, W_1 and W_2 are centred Brownian motions with diffusion coefficients and correlation, respectively,

$$\sigma_1 := \frac{2^{3/4}}{\sqrt{3}}, \quad \sigma_2 := \frac{1}{2^{1/4}}, \quad \rho := \frac{\sqrt{3}}{2}. \tag{13}$$

Notably, $\rho = \sigma_2/\sigma_1$, which implies that the process $\boldsymbol{W}$ satisfies the identity $2W_2 - W_1 \stackrel{d}{=} W_1$, which has a pre-limit analogue $2\widetilde{L} - \widetilde{X} \stackrel{d}{=} \widetilde{X}$. The identity can be explained by symmetry of the uniform distribution about $1/2$, which allows us to write

$$X(t) \stackrel{d}{=} \sqrt{\frac{2}{\nu}} \sum_{i=0}^{L(t)} (1 - U_i) = \sqrt{\frac{2}{\nu}}\, L(t) - X(t)\,.$$

The martingale (6) just coincides with the naturally centred L.

2.3 Self-similar asymptotically optimal strategies

We call strategy *self-similar* if the control $\psi = \psi_\nu$ has the form

$$\psi(t,x) := (1-x)\delta(\nu(1-t)(1-x)), \quad (t,x) \in [0,1]^2. \tag{14}$$

for some function $\delta : \mathbb{R}_+ \to [0,1]$. Note that such a strategy is feasible and $\psi_\nu(0,0) = \delta(\nu)$. The rationale behind this definition is the following. Assuming x to be the running maximum at time t, the remaining part of the chain should be selected from the north-east rectangle spanned on (t,x) and $(1,1)$, and by the optimality principle the subsequence selected from the rectangle should have maximal expected length. Mapping the rectangle onto $[0,1]^2$ it is readily seen that the subproblem is an independent replica of the original problem of optimal selection from the unit square with intensity parameter $\nu(1-t)(1-x)$. The martingale (6) assumes the form

$$M(t) = L(t) + F(\nu(1-t)(1-X(t)) - F(\nu), \tag{15}$$

where the *value function* F, for given control, depends on one variable

$$F(\nu) := \mathbb{E}L_\nu(1), \quad F(0) = 0.$$

Assumption. From this point on we assume that *the selection strategy is self-similar as defined by* (14)*, with function δ having asymptotics*

$$\delta(\nu) = \sqrt{2/\nu} + O\left(\nu^{-1}\right), \quad \nu \to \infty. \tag{16}$$

The assumption is central and deserves comments. Whenever $\nu(1-x)(1-t)$ is large, (16) implies asymptotics of the control

$$\psi(t,x) \sim \sqrt{\frac{2(1-x)}{\nu(1-t)}}, \tag{17}$$

which shows that near the diagonal $x = t$ the acceptance window is about the same as for the stationary strategy. Away from the diagonal the acceptance window is close to that for the stationary strategy adjusted to the rectangle north-east of (t, x).

It is known [11] that the optimal strategy satisfies the asymptotic expansion

$$\delta^*(\nu) \sim \sqrt{2/\nu} - (3\nu)^{-1} + O(\nu^{-3/2}). \tag{18}$$

A minor adjustment of Theorem 6 in [11] shows that if we assume, more generally, the relation $\delta(\nu) \sim \sqrt{2/\nu} + \beta/\nu$ with some parameter $\beta \in \mathbb{R}$, then asymptotic expansions of the moments (1), (2) are still valid, with only constant terms depending on β. Using a sandwich argument based on Lemma 1, it can be further shown that under the assumption (16) expansions of the moments hold but with constant terms being replaced by some $O(1)$ remainders. In particular, condition (16) ensures the two-term asymptotic optimality (11), equivalent to the asymptotic expansion of the value function,

$$F(\nu) = \sqrt{2\nu} - \frac{1}{12}\log(\nu + 1) + O(1). \tag{19}$$

We stress that the logarithmic term here (as well as in the counterpart of the variance formula (2)) is not affected by the remainder in (16), rather appears due to the self-similar adjustment of the (feasible version of) stationary strategy, as incorporated in (17).

Approximation (17) is not useful when t or x are too close to 1, so that $\nu(1-t)(1-x)$ varies within $O(1)$. To embrace the full range of the variables, for the sequel we choose $\beta > 1$ large enough to meet the bounds

$$\left|\psi(t, x) - \sqrt{\frac{2(1-x)}{\nu(1-t)}}\right| \quad < \quad \frac{\beta}{\nu(1-t)}, \quad \text{for} \quad (t, x) \in [0, 1) \times [0, 1). \tag{20}$$

This will be employed along with the bound

$$\psi(t, x) \quad < \quad \frac{1}{\nu(1-t)}, \quad \text{for} \quad 1 - x < \frac{1}{\nu(1-t)} \tag{21}$$

which follows by feasibility.

3 Generators

A major technical difficulty in showing the convergence in $D[0, 1]$ is the singularity of (17) at $t = 1$. This will be handled in two steps. First, we bound the time variable away from $t = 1$ and show the convergence of the generators on a sufficiently big space of test functions. Then we will apply domination arguments to bound fluctuations near the right endpoint, thus justifying convergence on the full $[0, 1]$.

The processes we consider are not time-homogeneous, therefore by computing generators we include the time variable in the state vector. From (4), the generator of the jump process (X, L) is

$$\mathcal{L}_\nu f(t, x, \ell) = f_t(t, x, \ell) + \nu \int_0^{\psi(t,x)} \{f(t, x + u, \ell + 1) - f(t, x, \ell)\}\mathrm{d}u.$$

For the processes centered by t we should include $-f_x - f_\ell$ in the generator. Then, with the change of variables

$$x \to x\nu^{-1/4} + t, \;\; \ell \to (\ell\nu^{-1/4} + t)\sqrt{2\nu}, \;\;\; \widetilde{\psi}(t, x) := \nu^{1/4}\psi(t, x\nu^{-1/4} + t)$$

we arrive at the generator of $(\widetilde{X}, \widetilde{L})$

$$\widetilde{\mathcal{L}}_\nu f = f_t - \nu^{1/4}(f_x + f_\ell) + \nu^{3/4} \int_0^{\widetilde{\psi}(t,x)} \{f(t, x+u, \ell+v) - f(t, x, \ell)\}\mathrm{d}u, \tag{22}$$

where we abbreviate $f = f(t, x, \ell)$ etc., and

$$v := (4\nu)^{-1/4} \tag{23}$$

We extend $\widetilde{\mathcal{L}}_\nu f$ by 0 outside the reachable range of $(\widetilde{X}, \widetilde{L})$. Note that the range of $\widetilde{X}(t)$ lies within the bounds

$$-t\nu^{1/4} \le x \le (1-t)\nu^{1/4}.$$

We fix $h \in (0,1)$ and focus on $t \in [0, 1-h]$, so achieving uniformly in this range

$$\widetilde{\psi}(t, x) = O(\nu^{-1/4}), \tag{24}$$

and for $k \ge 1$

$$\widetilde{\psi}^k(t, x) = \left(2 - \frac{2x}{\nu^{1/4}(1-t)}\right)^{k/2} \nu^{-k/4} + O(\nu^{-(k+2)/4}), \text{ for } x \le (1-t)\nu^{1/4} - \frac{1}{\nu^{3/4}(1-t)} \tag{25}$$

as dictated by the bounds (20), (21).

Now let $\mathcal{D}$ be the space of vanishing at infinity functions $f \in C_0^3([0,1] \times \mathbb{R}^2)$ which satisfy a rapid decrease property

$$\sup |x^k f_\bullet(t, x, \ell)| < \infty,$$

where $f_\bullet$ is any derivative of f of the first or second order and $k > 0$. Set

$$D^{>}_{h,\nu} := \{(t, x, \ell) : t \in [0, 1-h],\ |x| > \nu^{1/16}\}, \quad D^{<}_{h,\nu} := \{(t, x, \ell) : t \in [0, 1-h],\ |x| \le \nu^{1/16}\}.$$

We shall be using that for $f \in \mathcal{D}$

$$\lim_{\nu \to \infty} \sup_{D^{>}_{h,\nu}} |\nu^k f_\bullet(x)| = 0. \tag{26}$$

The integrand in (22) expands as

$$f(t, x+u, \ell+v) - f(t, x, \ell) = f_x u + f_\ell v + \frac{1}{2} f_{xx}\, u^2 + f_{x\ell}\, uv + \frac{1}{2} f_{\ell\ell}\, v^2 + R,$$

where the remainder can be estimated as

$$|R| \le c \sum_{i=0}^{3} u^i v^{3-i},$$

with constant c chosen bigger than the maximum absolute value of any third derivative of f. Hence for the integrated remainder we have a uniform estimate

$$\nu^{3/4} \left| \int_0^{\widetilde{\psi}} R du \right| \le \nu^{3/4} c \sum_{i=1}^{4} \widetilde{\psi}^i v^{4-i} = O(\nu^{-1/4}),$$

using (24), (23).

Integrating the Taylor polynomial yields

$$\widetilde{\mathcal{L}}_\nu f = f_t - \nu^{1/4}(f_x + f_\ell) + \nu^{3/4}\left\{\frac{f_x\,\widetilde{\psi}^2}{2} + f_\ell\, v\widetilde{\psi} + \frac{f_{xx}\widetilde{\psi}^3}{6} + \frac{f_{x\ell}\,\widetilde{\psi}^2}{2}v + \frac{f_{\ell\ell}v^2\widetilde{\psi}}{2}\right\} + O(\nu^{-1/4}).$$

Applying (26)

$$\lim_{\nu\to\infty}\sup_{D^{>}_{h,\nu}} |\widetilde{\mathcal{L}}_\nu f(t,x,\ell)| = 0. \tag{27}$$

Thus we focus on the range $D^{<}_{h,\nu}$, where (20) and (25) can be employed. From (20)

$$-\nu^{1/4} f_x + \nu^{3/4}\frac{1}{2}f_x\widetilde{\psi}^2 = -\frac{x}{1-t}f_x + O(\nu^{-1/4}).$$

Observing that in this range $|x\nu^{-1/4}| \le \nu^{-3/16}$ for $k > 0$ we expand as

$$\widetilde{\psi}^k(t,x,\ell) = 2^{k/2}\nu^{-k/4} - \frac{2^{k/2-1}x}{1-t}\nu^{-(k+1)/4} + O(\nu^{-(k+1)/4-1/8}),$$

with the remainder estimate being uniform over $D^{<}_{h,\nu}$. The remaining calculations is a careful book-keeping using this formula and that the derivatives are uniformly bounded.

Define operator

$$\widetilde{\mathcal{L}}f := f_t - \frac{x}{1-t}f_x - \frac{x}{2(1-t)}f_\ell + \frac{{\sigma_1}^2}{2}f_{xx} + \frac{{\sigma_2}^2}{2}f_{\ell\ell} + \sigma_1\sigma_2\rho f_{x\ell},$$

with σ_1, σ_2, and ρ given by (13).

▶ **Lemma 2.** *For $f \in \mathcal{D}$ and $h \in (0,1)$*

$$\lim_{\nu\to\infty}\sup_{(t,x,\ell)\in[0,1-h]\times\mathbb{R}^2} |\widetilde{\mathcal{L}}_\nu f(t,x,\ell) - \widetilde{\mathcal{L}}f(t,x,\ell)| = 0.$$

Operator $\widetilde{\mathcal{L}}$ is the generator of a Gaussian diffusion process which satisfies the stochastic differential equation

$$\mathrm{d}Y_1(t) = -\frac{Y_1(t)}{1-t}\,\mathrm{d}t + \mathrm{d}W_1(t), \tag{28}$$

$$\mathrm{d}Y_2(t) = -\frac{Y_1(t)}{2(1-t)}\,\mathrm{d}t + \mathrm{d}W_2(t), \tag{29}$$

with zero initial value, where $\boldsymbol{W} = (W_1, W_2)$ is the two-dimensional Brownian motion with covariance $\boldsymbol{\Sigma}$ introduced in (12).

From the equation for the first component (28), it is seen that Y_1 is a Brownian bridge

$$Y_1(t) = (1-t)\int_0^t \frac{\mathrm{d}W_1(s)}{1-s}, \tag{30}$$

with the covariance function $\mathrm{Cov}(Y_1(s), Y_1(t)) = \sigma_1 s(1-t)$, $0 \le s \le t \le 1$. In particular, $Y_1(1) = 0$. We shall discuss the second component later on.

The space $\mathcal{D}$ is dense in a larger space $C^3_0([0,1-h]\times\mathbb{R}^2)$. Since the differentiability properties of functions are preserved under averaging over normally distributed translations, $\mathcal{D}$ is invariant under the semigroup of $\boldsymbol{Y}$. Thus by Watanabe's theorem (see [13], Proposition

17.9) $\mathcal{D}$ is a core of operator $\widetilde{\mathcal{L}}$. The above Lemma 2 and Theorem 17.25 from [13] now imply weak convergence

$$(\widetilde{X}_\nu, \widetilde{L}_\nu) \Rightarrow (Y_1, Y_2) \ \text{ in } \ D[0, 1-h] \tag{31}$$

for every $h \in (0,1)$. A closer inspection of the above approximation errors suggests that the quality of convergence deteriorates as $h \to 0$.

We encountered the Brownian motion $\boldsymbol{W}$ in connection with the free-endpoint stationary strategy in Section 2.2. Now we see that the variable control (17) causes a drift that forces the running maximum to timely arrive at the north-east corner of the square.

4 The functional limit in $D[0,1]$

The martingale problem for $\widetilde{\mathcal{L}}$ is well-posed on the complete interval, and the SDE (28) has a unique strong solution. This suggests to extend convergence (31) to the full $[0,1]$. To that end, we need to monitor the behaviour of $\widetilde{\mathcal{L}}_\nu f$ for t close to 1.

Since (31) entails convergence of finite-dimensional distributions for times $t < 1$ and ensures that the modulus of continuity behaves properly over $[0, 1-h]$, to justify tightness of $\widetilde{X}_\nu$'s, and hence their convergence on $[0,1]$, it will be enough to show that

$$\lim_{h\to 0} \limsup_{\nu} \mathbb{P}(\sup_{t\in[1-h,1]} |\widetilde{X}_\nu(t)| > h^{1/4}) = 0. \tag{32}$$

Define $\xi_{\nu,h}$ by setting

$$\widetilde{X}_\nu(1-h) = \sigma_1 \sqrt{h(1-h)}\, \xi_{\nu,h}.$$

Since $\widetilde{X}_\nu(1-h) \stackrel{d}{\to} Y_1(1-h)$ the distribution of $\xi_{\nu,h}$ is close to $\mathcal{N}(0,1)$ for large ν.

By self-similarity of the selection strategy, $((X_\nu(t)-t),\ t \in [1-h,1])$ has the same distribution as $(h^{-1}(X_{\nu h^2}(t)-t),\ t \in [0,1])$ with the initial value $X_{\nu h^2}(0) = \nu^{-1/4}\sigma_1\sqrt{(1-h)/h}\,\xi_{\nu,h}$, as is seen by zooming in the corner square north-east of the point $(1-h, 1-h)$ with factor h^{-1}. Changing variable $\nu h^2 \to \nu$, (32) translates as a compact containment condition

$$\lim_{h\to 0} \limsup_{\nu} \mathbb{P}(\sup_{t\in[0,1]} |\widetilde{X}_\nu(t)| > h^{-1/4}) = 0 \tag{33}$$

under the initial value $\widetilde{X}_\nu(0) = \sqrt{1-h}\,\xi_{\nu,h}$.

To verify (33) we shall squeeze the running maximum X between $X^\downarrow$ and $X^\uparrow$ whose normalised versions satisfy the compact containment condition. We force the majorant and the minorant to live on the opposite sides of the diagonal. Both have independent, almost stationary increments, so that functional limits can be readily identified. For simplicity we will assume $X_\nu(0) = 0$. The general case with $X_\nu(0)$ of the order $\nu^{-1/4}$ can be handled by the same method.

4.1 Majorant

Define process $X^\uparrow = X^\uparrow_\nu$ as solution to

$$\mathrm{d}X^\uparrow(t) = \int_0^{\psi^\uparrow(t)} x\Pi^*(\mathrm{d}t\mathrm{d}x) + 1(X^\uparrow(t) = t)\mathrm{d}t,$$

$X^{\uparrow}(0) = K\nu^{-1/2}$ for some big enough $K > 0$, with control

$$\psi^{\uparrow}(t) := \sqrt{\frac{2}{\nu}} + \frac{\beta}{\nu(1-t)} 1(t \le 1 - K\nu^{-1/2})$$

not depending on x. Notation $1(\cdots)$ is used for indicators. The process never drops below the line $x = K\nu^{-1/2} + t$, and whenever the line is hit the path drifts along it for some time. By the construction, above the diagonal the process $X^{\uparrow}$ increases faster than X, and is, in fact, a majorant.

▶ **Lemma 3.** *By coupling via* (4), $X^{\uparrow} \ge X$ *a.s.*

Let

$$S(t) := \int_0^t \int_0^{\psi^{\uparrow}(t)} x\Pi^*(\mathrm{d}s\mathrm{d}x) - t.$$

This is a process with independent increments, which we can split in two independent components

$$S(t) = \left(\int_0^t \int_0^{\sqrt{2/\nu}} x\Pi^*(\mathrm{d}s\mathrm{d}x) - t \right) + \int_0^t \int_{\sqrt{2/\nu}}^{\psi^{\uparrow}(t)} x\Pi^*(\mathrm{d}s\mathrm{d}x).$$

The mean value of the second part is estimated as

$$\frac{2\nu}{\sqrt{\nu}} \int_0^{1-K/\sqrt{\nu}} \frac{\beta}{\nu(1-t)} \mathrm{d}t = O\left(\frac{\log \nu}{\sqrt{\nu}}\right),$$

and the first is a compensated compound Poisson process. Thus $\nu^{1/4} S \Rightarrow W_1$ as $\nu \to \infty$.

Processes akin to $(X^{\uparrow}(t) - t,\ t \in [0,1])$ are common in applied probability [3, 5]. In particular, by the interpretation as the content of a single-server M/G/1 queue, the positive increments present jobs that arrive by Poisson process and are measured in terms of the demand on the service time. The downward drift occurs due to the unit processing rate when the server is busy. Borrowing a useful identity,

$$X^{\uparrow}(t) - t = S(t) - \inf_{u \in [0,t]} S(u),$$

we conclude on the weak convergence $(\nu^{1/4}(X^{\uparrow}(t) - t),\ t \in [0,1]) \Rightarrow |W_1|$ to a reflected Brownian motion.

4.2 Minorant

$$\psi^{\downarrow}(t,x) = \begin{cases} \left(\sqrt{\frac{2}{\nu}} - \frac{\beta}{\nu(1-t)}\right) \wedge (t-x), & \text{for} \quad 0 \le t \le 1 - K/\sqrt{\nu}, \\ 0, \quad \text{for} \quad 1 - K/\sqrt{\nu} < t \le 1. \end{cases}$$

where K is sufficiently large. We can regard this as a suboptimal strategy that never selects marks $x > t$. Starting at state 0, the running maximum process stays below the diagonal throughout, and gets frozen at $t = 1 - K/\sqrt{\nu}$. A counterpart of Lemma 3, $X^{\downarrow} < X$ a.s., is readily checked.

Switching general $\beta > 0$ to $\beta = 0$ impacts $\mathbb{E}X^{\downarrow}(t)$ by $O(\nu^{-1/2}\log \nu)$ uniformly in $t \in [0,1]$. Indeed, the jumps are bounded by $2/\sqrt{\nu}$, and the expected number of jumps increases by $O(\log \nu)$.

Assuming $\beta = 0$, the process $(X^{\downarrow}(t) - t,\ t \in [0, 1 - K\nu^{-1/2}])$ is a compensated compound Poisson process on the negative halfline, with reflection at 0. We have therefore

$$(\nu^{1/4}(X^{\downarrow}(t) - t),\ t \in [0,1]) \Rightarrow -|W_1|.$$

A rigorous proof can be obtained by inspecting convergence of the generator acting on the functions $f \in \mathcal{D}$ with $f_x(t, 0) = 0$.

4.3 The length process near termination

Having established weak convergence of $\widetilde{X}$, the fluctuations of $\widetilde{L}$ near $t = 1$ are estimated by verifying that

$$\lim_{h\to 0} \limsup_{\nu} \mathbb{P}(\sup_{t\in[1-h,1]} |\widetilde{L}(t) - \widetilde{L}(1-h)| > \epsilon) = 0. \tag{34}$$

This is done with the help of analysis of the martingale M.

5 Main result

By the domination argument, tightness of $(\widetilde{X}_\nu, \widetilde{L}_\nu)$ follows on the whole $[0, 1]$, and we arrive at our main result.

▶ **Theorem 4.** *The normalised running maximum and the length process* (3) *driven by a control satisfying* (14) *and* (16) *(in particular, under the optimal online selection strategy) converge weakly in the Skorokhod space $D[0, 1]$,*

$$(\widetilde{X}_\nu, \widetilde{L}_\nu) \Rightarrow (Y_1, Y_2), \quad \text{as} \quad \nu \to \infty,$$

where the limit bivariate process is a Gaussian diffusion defined by the equations (28), (29) *with zero initial conditions.*

We observed already that Y_1 is the Brownian bridge (30) and from (29)

$$Y_2(t) = \frac{Y_1(t)}{2} - \frac{W_1(t)}{2} + W_2(t),$$

so splitting the martingale part in independent components, we get, explicitly,

$$Y_2(t) = \int_0^t \frac{(1-t)}{2(1-s)} \mathrm{d}W_1(s) + \frac{1}{4}\, W_1(t) + \left(W_2(t) - \frac{3}{4}\, W_1(t) \right), \tag{35}$$

which is a sum of a Brownian motion, derived Brownian bridge and another independent Brownian motion.

To find the covariance structure, it is convenient to resort to matrix calculations. We may write the solution to (28), (29) as

$$\boldsymbol{Y}(t)^T = e^{a(t)} \int_0^t e^{-a(u)} \mathrm{d}\boldsymbol{W}(u)^T,$$

where

$$a(t) := A \int_0^t \frac{1}{1-u} \mathrm{d}u = A \log(1-t), \qquad A := \begin{pmatrix} 1 & 0 \\ \frac{1}{2} & 0 \end{pmatrix},$$

which yields by the Itó isometry

$$\mathbb{E}\{\boldsymbol{Y}(s)^T\boldsymbol{Y}(t)\} = \int_0^t e^{a(s)-a(u)}\boldsymbol{\Sigma} e^{(a(t)-a(u))^T}\mathrm{d}u, \qquad 0 \le s \le t \le 1.$$

Since A is idempotent matrix, the exponents are readily calculated as

$$e^{a(t)} = \begin{pmatrix} 1-t & 0 \\ -\frac{t}{2} & 1 \end{pmatrix}, \qquad e^{-a(t)} = \begin{pmatrix} \frac{1}{1-t} & 0 \\ \frac{t}{2(1-t)} & 1 \end{pmatrix},$$

and we arrive at the cross-covariance matrix

$$\mathbb{E}\{\boldsymbol{Y}(s)^T\boldsymbol{Y}(t)\} \;=\; \begin{pmatrix} \frac{2\sqrt{2}\,s(1-t)}{3} & \frac{2s(1-t)-(1-s)\log(1-s)}{3\sqrt{2}} \\ \frac{(1-t)(2s-\log(1-s))}{3\sqrt{2}} & \frac{2s(2-t)-(2-s-t)\log(1-s))}{6\sqrt{2}} \end{pmatrix},$$

where $0 \le s \le t \le 1$.

The limit length process Y_2 is *not* Markovian, since its covariance function does not satisfy the factorisation criterion (see [14], p. 148). The sum of two first terms in (35) is non-Markovian too.

6 Diffusion approximation in the bin-packing problem

We turn to a version of the bin-packing problem. Suppose that i.i.d., positive marks arrive by a Poisson process of intensity ν on $[0,1]$, and that the marks are sampled from a density satisfying $f(y) \sim A\alpha y^{\alpha-1}$ as $y \to 0$, with $\alpha, A > 0$. The stochastic optimisation task is to maximise the expected number of online selections under the constraint that their total does not exceed given $c > 0$.

Let $Z_\nu(t), N_\nu(t)$, $t \in [0,1]$ denote the sum and the number of selected marks at time t under the optimal selection policy, which has a control function $\psi(t,z) = (c-z)\,\delta(\nu(1-t)(c-z)^\alpha)$, where

$$\delta(\nu) = \frac{\gamma_1}{\nu^{1/(\alpha+1)}} + O(\nu^{-2/(\alpha+1)}), \quad \nu \to \infty, \;\gamma_1 = \left(\frac{(\alpha+1)}{A\,\alpha}\right)^{1/(\alpha+1)},$$

see [9]. It was shown in [9] that the mean number of selections has asymptotics $u(\nu) \sim \gamma_2\,\nu^{1/(\alpha+1)}$, $\nu \to \infty$, with

$$\gamma_2 = \left(\frac{c(\alpha+1)}{A\,\alpha}\right)^{1/(\alpha+1)}.$$

This suggests the normalisations

$$\widetilde{Z}_\nu(t) := \nu^{1/(2(\alpha+1))}\,(Z_\nu(t) - ct)\,, \quad \widetilde{N}_\nu(t) := \nu^{1/(2(\alpha+1))}\left(\frac{N_\nu(t)}{\gamma_2\nu^{1/(\alpha+1)}} - t\right).$$

The infinitesimal generator of $(t, \widetilde{Z}_\nu(t), \widetilde{N}_\nu(t))$ is

$$\mathcal{L}_\nu f(t,z,n) = f_t - \nu^{1/(\alpha+1)}(cf_z + f_n) \\ + \nu^{1-1/(2(\alpha+1))}\int_0^{\widetilde{\psi}(t,z)}\left(f\left(t, z+y, n+\frac{1}{\gamma_2\nu^{1/(2(\alpha+1))}}\right) - f(t,z,n)\right) f(y)\mathrm{d}y,$$

where

$$\widetilde{\psi}(t,z) = \nu^{1/(2(\alpha+1))}\,\psi(t, z\nu^{-1/(2(\alpha+1))} + tc).$$

A fairly long computation yields the asymptotics, as $\nu \to \infty$,

$$\mathcal{L}_\nu f(t,z,n) \sim f_t - \frac{z}{1-t} f_z - \frac{\alpha z}{c(\alpha+1)(1-t)} f_n + \frac{{\sigma_3}^2}{2} f_{zz} + \frac{{\sigma_4}^2}{2} f_{nn} + \rho_0 \sigma_3 \sigma_4 f_{zn},$$

where

$$\sigma_3 = \frac{(\alpha+1)^{(\alpha+2)/(2(\alpha+1))}\sqrt{c}}{\sqrt{\alpha+2}}, \ \sigma_4 = \frac{1}{A^{1/(2(\alpha+1))}(\alpha+1)^{\alpha/(2(\alpha+1))}},$$

and

$$\rho_0 = \frac{\alpha^{\alpha/(\alpha+1)}\sqrt{\alpha+2}}{c^{(\alpha-1)/(2(\alpha+1))}A^{\alpha/(2(\alpha+1))}(\alpha+1)^{2\alpha/(\alpha+1)}}.$$

Using this we were able to show the functional convergence

$$(\widetilde{Z}_\nu, \widetilde{N}_\nu) \Rightarrow (Y_3, Y_4), \quad \text{as} \ \ \nu \to \infty,$$

in $D[0,1-h]$ for every $h \in (0,1)$, where the limit process $(Y_3(t), Y_3(t))$ is a Gaussian diffusion satisfying the SDE

$$\mathrm{d}Y_3(t) = -\frac{Y_3(t)}{1-t}\,\mathrm{d}t \ + \mathrm{d}W_3(t), \quad \mathrm{d}Y_4(t) = -\frac{\alpha Y_3(t)}{c(\alpha+1)(1-t)}\,\mathrm{d}t \ + \mathrm{d}W_4(t)$$

with zero initial conditions. Here, (W_3, W_4) is a two-dimensional centred Brownian motion with the covariance matrix $\mathbf{\Sigma_0} = \begin{pmatrix} {\sigma_3}^2 & \rho_0\sigma_3\sigma_4 \\ \rho_0\sigma_3\sigma_4 & {\sigma_4}^2 \end{pmatrix}$.

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Analysis of Lempel-Ziv'78 for Markov Sources

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Abstract

Lempel-Ziv'78 is one of the most popular data compression algorithms. Over the last few decades fascinating properties of LZ78 were uncovered. Among others, in 1995 we settled the Ziv conjecture by proving that for a *memoryless source* the number of LZ78 phrases satisfies the Central Limit Theorem (CLT). Since then the quest commenced to extend it to Markov sources. However, despite several attempts this problem is still open. The 1995 proof of the Ziv conjecture was based on two models: In the DST-model, the associated digital search tree (DST) is built over m *independent* strings. In the LZ-model a *single* string of length n is partitioned into variable length phrases such that the next phrase is not seen in the past as a phrase. The Ziv conjecture for memoryless source was settled by proving that both DST-model and the LZ-model are asymptotically equivalent. The main result of this paper shows that this is not the case for the LZ78 algorithm over Markov sources. In addition, we develop here a large deviation for the number of phrases in the LZ78 and give a *precise* asymptotic expression for the redundancy which is the excess of LZ78 code over the entropy of the source. We establish these findings using a combination of combinatorial and analytic tools. In particular, to handle the strong dependency between Markov phrases, we introduce and precisely analyze the so called *tail symbol* which is the first symbol of the next phrase in the LZ78 parsing.

2012 ACM Subject Classification Mathematics of computing → Information theory

Keywords and phrases Lempel-Ziv algorithm, digital search trees, depoissonization, analytic combinatorics, large deviations

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.15

Funding *Wojciech Szpankowski*: This work was supported by NSF Center for Science of Information (CSoI) Grant CCF-0939370, and in addition by NSF Grant CCF-1524312.

Acknowledgements We thank Guillaume Duboc for simulation of LZ78 scheme resulting in Figure 2.

1 Introduction

The Lempel-Ziv compression algorithm [16] is a universal compression scheme. It partitions the text to be compressed into consecutive phrases such that the next phrase is the unique shortest prefix (of the uncompressed text) not seen before as a phrase. For example, $aababbababbb$ is parsed as $()(a)(ab)(abb)(aba)(b)(bb)$. The LZ78 compression code consists of a pointer to the previous phrase and the last symbol of the current phrase. The distribution of the number of phrases and other related quantities (such as redundancy and code length) are known for memoryless sources [10, 14] but research over the past 40 years has failed to produce any significant progress for Markov sources. In this paper, we present novel large deviations and precise redundancy results that had been wanting since the algorithm inception, as well as some surprising findings regarding the difference between the memoryless case and the Markov case.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 15; pp. 15:1–15:19
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

It is convenient to organize phrases (dictionary) of the Lempel-Ziv scheme in a *digital search tree* (DST) [6] which represents a parsing tree. We assume throughout that $\mathcal{A} = \{a, b\}$. Then the root contains an empty phrase. The first phrase is the first symbol, say "$a \in \mathcal{A}$" which is stored in a node appended to the root. The next phrase is either $(aa) \in \mathcal{A}^2$ stored in another node that branches out from the node containing the first phrase "a" or (ab) that is stored in a node attached to the root. This process repeats recursively until the text is parsed into full phrases (see Figure 1). A detailed description can be found in [3, 6, 8].

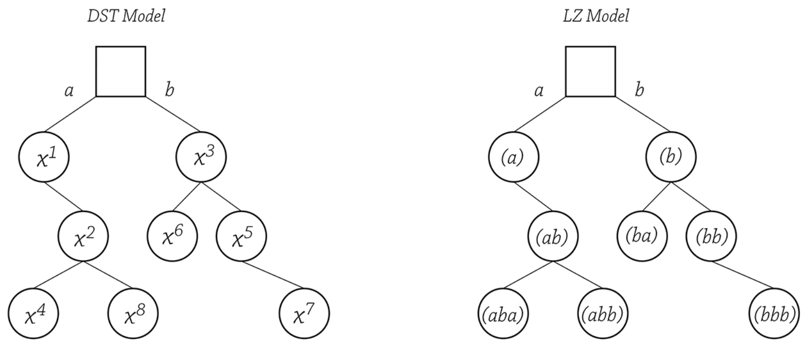

Figure 1 The DST-model vs LZ-model. In the DST-model we inserted eight (infinite) strings: $X^1 = a\mathbf{b}b\cdots$, $X^2 = ab\mathbf{b}\cdots$, $X^3 = bb\mathbf{ba}\cdots$, $X^4 = aba\mathbf{aa}\cdots$, $X^5 = bb\mathbf{aa}\cdots$, $X^6 = ba\mathbf{aa}\cdots$, $X^7 = bbb\mathbf{a}\cdots$ and $X^8 = abb\mathbf{bb}\cdots$, where bold symbols denote DST tail symbols. In the LZ-model we parsed one string $X = ()(a)(\mathbf{a}b)(\mathbf{b})(\mathbf{a}aba)(\mathbf{b}b)(\mathbf{b}bb)(\mathbf{a}bb)$ with bold denoting LZ tail symbols.

We consider two models called the DST-model and the LZ-model. In the DST-model we insert *independent strings* although each string may be generated by a source with memory like a Markov source. In the LZ-model we parse a *single* string as shown in Figure 1. We distinguish two types of DST and LZ models. To define them we need to introduce the path length L as the sum of all depths in the digital search tree or the sum of all phrases in the LZ model. In the "m"-DST model we insert m independent strings into a digital search tree – leading to a variable path length denoted as L_m – while the "n"-DST model is built over a random number of independent strings such that the total path length is equal to n. Similarly, we have "m"-LZ and "n"-LZ models: In the former we construct m LZ phrases to form a string of (variable) length denoted as $\mathcal{L}_m$ while in the "n"-LZ model we parse a string of length n into a variable number of phrases that we denote as M_n. Throughout, m will denote number of strings or phrases while n will stand for the length of a string.

There is a simple relation between M_n and $\mathcal{L}_m$ called the *renewal equation* which asserts

$$P(M_n > m) = P(\mathcal{L}_m < n). \tag{1}$$

Finally, observe that the code length of the LZ78 algorithm is $C_n = \sum_{k=1}^{M_n} \lceil \log_2(k) \rceil + \lceil \log_2(|\mathcal{A}|) \rceil$ since the pointer to the kth node requires at most $\lceil \log_2 k \rceil$ bits, while the next symbol costs $\lceil \log_2 |\mathcal{A}| \rceil$ bits. For binary alphabet $\mathcal{A} = \{a, b\}$ we simplify the code length to $C_n = M_n (\log_2 M_n + 1)$.

To understand LZ78 behavior one must analyze the limiting distribution of M_n and/or $\mathcal{L}_m$ connected through the renewal equation (1). For *memoryless* sources we benefited from the fact the random variable L_m and $\mathcal{L}_m$ are *probabilistically equivalent* as shown in 1995 paper [3]. Unfortunately, this equivalence breaks for sources with memory such as Markov sources. To capture this dependency we introduce the notion of the *tail symbol*. In the

DST-model the tail symbol of an inserted string is the first non-inserted symbol of that string, as shown in Figure 1. In the LZ-model the tail symbol of a phrase is the first symbol of the next phrase (see Figure 1). Furthermore, in the Markov case there is additional complication, even for the DST-model. In the DST-model we need to consider two digital search trees: one built over all (independent) strings starting with symbol $a \in \mathcal{A}$, and the second one built over all strings that start with $b \in \mathcal{A}$. At the end we construct a cumulative knowledge by weighting over the initial symbols (see [7]).

In this paper, we present large deviation results for the number of phrases M_n in "n"-LZ model and the average length of a LZ (Markov) string built over m phrases in the "m"-LZ model.[1] In the memoryless case we could read the number of phrases M_n directly from the path length L_m of the m-DST model. It is *not* the case in the Markov model but through the tail symbol distribution we will connect both quantities. Recall that $\mathcal{L}_m$ is the length of a string generated by a Markov source which is parsed by the LZ78 scheme until we see m phrases (our m-LZ model). This should be compared to the total path length L_m (notice roman font for L) in the the m-DST model. In the memoryless case, we proved in [3, 5] that the expected value of L_m and the expected value of the length of a string built from m phrases, $\mathcal{L}_m$, are the same. Somewhat surprisingly it is not the case for the Markov case. We will prove in Theorem 5 that $\mathbf{E}[L_m] - \mathbf{E}[\mathcal{L}_m] = \Theta(m)$.

Let us now briefly review literature on LZ78 and DST analysis. The goal is to prove the Central Limit Theorem (CLT) for the number of phrases and establish precise rate of decay of the LZ78 code redundancy for Markov sources. For memoryless sources, CLT was already proved in [3] while the average redundancy was presented in [10, 14]. It should be pointed out that since 1995 paper [3] no simpler, in fact, no new proof of CLT was presented except the one by Neininger and Rüschendorf [13] but only for *unbiased* memoryless sources (as in [1]). The only known to us analysis of LZ78 for Markov sources is presented in [7], but the authors restricted their attention to a single phrase. We should point out that for another Lempel-Ziv scheme known as LZ'77 algorithm, Fayolle and Ward [2] analyzed an associated suffix tree built over a Markov string and obtained the distribution of the depth, which allows us to conclude the limiting distribution of a phrase in the LZ'77 scheme (see also [11, 12]). Regarding analysis of digital search trees, and in general digital trees, more is known [8, 6, 15]. Digital trees for memoryless sources were analyzed in [1, 10, 6] while digital trees under Markovian models were studied in [7, 9, 2]. This information is surveyed in detail in [6].

The paper is organized as follows. In the next section we present our main results regarding the LZ and DST models including the mean, variance and distribution of the number of tail symbols in the DST model (see Theorem 2–4), and large deviations as well as precise redundancy for the LZ model (see Theorems 5–6). We prove these findings in Section 3 (DST model) and in Section 4 (LZ model), with most details delayed till the appendix. Throughout we use combinatorics on words and analytic tools such as generating functions, Poisson transform, analytic depoissonization, and Mellin transform.

2 Main Results

We consider a stationary ergodic Markov source generating a sequence of symbols drawn from a finite alphabet $\mathcal{A}$. In this paper we study only a binary Markovian process of order 1 with the transition matrix $\mathbf{P} = [P(c|d)]_{c,d \in \mathcal{A}}$ where $\mathcal{A} = \{a, b\}$. In this section we present our main results with proof delayed till Sections 3–4 and appendix. However, first we present a road map of our methodology and findings.

[1] From now on we drop the quotes around m and n to simplify the presentation.

Our main goal is to analyze the Lempel-Ziv'78 scheme for Markovian input. However, as discussed before, we first consider an auxiliary model named DST-model built over m independent Markov strings, also called the m-DST model. However, for Markov sources we need to construct two *conditional* digital search trees: one built over m Markov strings all starting with symbol $a \in \mathcal{A}$ and the other DST built over m strings starting with $b \in \mathcal{A}$. We write $c \in \mathcal{A}$ for a generic symbol from $\mathcal{A}$, that is, either $c = a$ or $c = b$. For a given $c \in \mathcal{A}$, we consider m independent Markov strings all starting with c and build an m-DST tree. For such a tree we analyze two quantities, namely the total path length denoted as L_m^c, and the number $T_m^c(a)$ of inserted strings (all starting with c) with the tail symbol a, that is, among m Markov strings there are $T_m^c(a)$ strings with the tail symbol a. Clearly, $T_m^c(a) + T_m^c(b) = m$. Throughout, we also assume that the tail symbol is always a so we just write $T_m^c := T_m^c(a)$. In Theorems 2-3 we summarize our new results regarding T_m^c, while in Theorem 4 we present large deviation results for both T_m^c and L_m^c.

Second, we consider the m-LZ model (in which we run LZ78 algorithm on a single string until we see m phrases) and tie it up to the m-DST model just discussed. Here we use a combinatorial approach. For a given sequence $\mathbf{s}$ over $\mathcal{A}$ of length m we compare in Lemmas 10-11 two probabilities: (i) the probability that in the m-LZ model (constructed from m LZ phrases) we end up with a LZ sequence of length n having all tail symbols equal to $\mathbf{s}$; and (ii) the probability that in the m-DST model (built over m independent Markov strings) the resulting digital search tree has path length equal to n and all tail symbols are equal to $\mathbf{s}$. Using this, we present in Theorem 5 our large deviations for the m-LZ model and using the renewal equation (1) in Theorem 6 we establish large deviations for the n-LZ model. In Corollary 7 we find a *precise* expression for the redundancy of LZ78 for Markov sources.

Finally, when comparing the average path length L_m^c in the m-DST model with the length $\mathcal{L}_m^c$ in the m-LZ model we shall use the following simple fact.

▶ **Proposition 1.** *For $\delta < 1$ let there exist $B, C > 0$ such that for a discrete random variable X_m the following holds uniformly*

$$P(X_m = k) \leq B \exp\left(-Cm^{-\delta}|k - A_m|\right). \tag{2}$$

Then

$$\boldsymbol{E}[X_m] = A_m + O(m^\delta). \tag{3}$$

Proof. Define $B_m = m^\delta(\log B)/C \leq |k - A_m|$. Then it is easy to see that $EX_m = \sum_k kP(X_m = k) = A_m + \sum_k (k - A_m)P(X_m = k)$, and the latter term can be estimated by the integral $2B\int_0^\infty \exp(-Cm^{-\delta}x)(x+1)dx = O(m^\delta)$. This completes the proof. ◀

2.1 Results on DST

In this section we summarize our results for the m-DST model: We first focus on the number of times, $T_m^c := T_m^c(a)$, the tail symbol is a when all m Markov sequences start with $c \in \mathcal{A}$. Then we study the path length L_m^c in the m-DST model when all sequences start with c. Finally, we present large deviations for both T_m^c and L_m^c.

For $c \in \mathcal{A}$, let $D_m^c(u) = E[u^{T_m^c}]$ be the probability generating function of T_m^c defined for a complex variable u. We have the recursion:

$$D_{m+1}^c(u) = (P(a|c)u + 1 - P(a|c)) \sum_k \binom{m}{k} P(a|c)^k P(b|c)^{m-k} D_k^a(u) D_{m-k}^b(u) \tag{4}$$

subject to $D_0^c(u) = 1$ and $D_1^c(u) = P(a|c)u + 1 - P(a|c)$. Furthermore, define the bivariate Poisson transform $D_c(z,u) = \sum_{m\geq 0} \mathbf{E}[u^{T_m^c}]\frac{z^m}{m!}e^{-z}$. From above we easily find the following differential-functional equation

$$\partial_z D_c(z,u) + D_c(z,u) = D_1^c(u) D_a(P(a|c)z,u)) \cdot D_b(P(b|c)z,u) \tag{5}$$

with $D_c(z,1) = 1$ where ∂_z is the partial derivative with respect to variable z.

We now focus on the first Poisson moment $X_c(z) = \partial_u D_c(z,1)$ where ∂_u is the derivative with respect to variable u. We also study the Poisson variance $V_c(z) = \partial_u^2 D_c(z,1) + X_c(z) - (X_c(z))^2$, and the limiting distribution of T_m^c. After finding the asymptotic behavior of the Poisson mean $X_c(z)$ and variance $V_c(z)$ for large $z \to \infty$ we invoke the depoissonization lemma of [4] to extract the original mean and variance:

$$\mathbf{E}[T_m^c] = X_c(m) - \frac{1}{2}m\partial_z X_c(m) + O(X_c(m)/m), \quad \mathrm{Var}[T_m^c] \sim V_c(m) - m[\partial_z X_c(m)]^2.$$

Let us start with the Poisson mean $X_c(z)$. Taking the derivative of (5) with respect to u and setting $u = 1$ we find

$$\partial_z X_c(z) + X_c(z) = P(a|c) + X_a(P(a|c)z) + X_b(P(b|c)z). \tag{6}$$

To complete this equation we need to calculate the initial values of $\mathbf{E}[T_m^c]$. It is easy to see that

$$\mathbf{E}[T_0^c] = 0, \quad \mathbf{E}[T_1^c] = P(a|c), \quad \mathbf{E}[T_2^c] = P(a|c) + P(a|c)P(a|a) + P(b|c)P(a|b). \tag{7}$$

In a similar fashion we can derive the differential-functional equation for the Poisson variance. After some tedious algebra we arrive at

$$\partial_z V_c(z) + V_c(z) = P(a|c) - P^2(a|c) + [\partial_z X_c(z)]^2 + V_a(P(a|c)z) + V_b(P(b|c)z). \tag{8}$$

Both differential-functional system of equations (5) and (7) can be solved using complicated Mellin transform approach [15]. We provide details of our approach in the Appendix. For now we need to introduce some extra notation to present our main results. For complex s define

$$\mathbf{P}(s) = \begin{bmatrix} P(a|a)^{-s} & P(b|a)^{-s} \\ P(a|b)^{-s} & P(b|b)^{-s} \end{bmatrix}. \tag{9}$$

For such $\mathbf{P}(s)$ we denote by $\lambda(s)$ the main eigenvalue and $\boldsymbol{\pi}(s)$ the main eigenvector. We notice that $\boldsymbol{\pi}(-1)$ is the stationary vector of the Markov process. We also need another matrix

$$\mathbf{Q}(s) = \prod_{i\geq 1}(\mathbf{I} - \mathbf{P}(s-i))^{-1} \prod_{j=-\infty}^{j=-2}(\mathbf{I} - \mathbf{P}(j))$$

defined for $\Re(s) \in (-2,0)$. Furthermore, $\langle \mathbf{x}, \mathbf{y} \rangle$ is the scalar product of vectors $\mathbf{x}$ and $\mathbf{y}$.

Now we are in the position to formulate our main result.

▶ **Theorem 2.** *Consider a digital search tree built over m independent sequences (m-DST) generated by a Markov source. We have $\boldsymbol{E}[T_m^c] = \tau_c(m)m$ and $\boldsymbol{E}[L_m^c] = m\log m/h + m + \mu_c(m)m$ such that:*
- *$\tau_c(m+1) - \tau_c(m) = O(1/m)$ and $\mu_c(m+1) - \mu_c(m) = O(1/m)$*
- *$\forall (c,d) \in \mathcal{A}^2$ $\tau_c(m) - \tau_d(m) = O(1/m)$ and $\mu_c(m) - \mu_d(m) = O(1/m)$.*

Thus $\tau_c(m) = \tau(m) + O(1/m)$ where $\tau(m)$ does not depend on initial symbol c. In fact, $\tau(m)$ depends on the tail symbol, but since throughout the paper we assume the tail symbol is always a, we drop this dependency on a in $\tau(m)$. We present precise formula on $\tau(m)$ in the next theorem.

Similarly we have $\mu_c(m) = \mu(m) + O(1/m)$. The function $\mu(m)$ for Markov sources is given in Theorem 1 of [7]. For the memoryless source, it is $\frac{h_2}{h} + \gamma - 1 + \alpha$ and the average path length is $m \log m/h + m\mu(m)$, as discussed in [3].

To complete our analysis of the tail symbol, we present now precise behaviour of $\tau(m)$. We give a detailed proof in the Appendix.

▶ **Theorem 3.** *For $(a, b, c) \in \mathcal{A}^3$ define*

$$\alpha_{abc} = \log \left[\frac{P(a|b)P(c|a)}{P(c|b)} \right]. \tag{10}$$

(i) Aperiodic case. *If not all $\{\alpha_{abc}\}$ are rational, then $\tau(m) = \bar{\tau} + o(1)$ with*

$$\bar{\tau} = \pi_a + \frac{1}{\lambda'(-1)} \langle \left(\boldsymbol{\pi}'(-1) + \boldsymbol{\pi} \boldsymbol{Q}'(-1) \right) (\boldsymbol{I} - \boldsymbol{P}) \boldsymbol{P} \boldsymbol{e}_a \rangle, \tag{11}$$

where π_a is the stationary distribution of symbol a, and $\boldsymbol{e}_a$ is the vector made of a single 1 at the position corresponding to symbol a and zero otherwise.

Periodic case. *If all $\{\alpha_{abc}\}$ are rationally related, then for some $\varepsilon > 0$ we have $\tau(m) = \bar{\tau}(m) + O(m^{-\varepsilon})$ with $\bar{\tau}(m) = \bar{\tau} + Q_1(\log m)$, where $Q_1(.)$ is a periodic function.*

(ii) Variance. *The variance $\mathrm{Var}[T_m^c]$ grows linearly, that is $\mathrm{Var}[T_m^c] \sim m\omega_a(m)$, where $\omega_a(m) = \bar{\omega}_a$ for the aperiodic case and $\omega_a(m) = \bar{\omega}_a + Q_2(m)$ for the periodic case, where $\bar{\omega}_a$ is given explicitly in the Appendix in (B.16) of Theorem 14, and $Q_2(m)$ is a nonzero periodic function for rationally related case, and zero otherwise.*

(iii) Central Limit Theorem. *For any $c \in \mathcal{A}$ we have*

$$\frac{T_m^c - \boldsymbol{E}[T_m^c]}{\mathrm{Var}[T_m^c]} \xrightarrow{d} N(0, 1)$$

where $N(0, 1)$ denotes the standard normal distribution.

Similarly we have the same behaviour for $\mu(m)$ which is equal to $\bar{\mu} + o(1)$ in the aperiodic case and, in the periodic case, is equal to $\bar{\mu} + Q_3(\log m) + O(m^{-\varepsilon})$ whose expressions are in [3] and [7] where $Q_3(.)$ is a periodic function. For details the reader is referred to [7].

We notice that, unexpectedly, the number of tail symbols equal to *a is not* converging to $n\pi_a$ as we should expect from a Markovian sequence. The reason is that the tail symbol is not picked up at random in the sequence but occurs when the sequence path leaves the tree.

Finally, we present joint large deviations for both T_m^c and L_m^c which is a new result needed to establish large deviations for the LZ model. We prove it in Section 3.

▶ **Theorem 4.** *Consider a digital search tree (DST) built over m independent sequences generated by a Markov source. For all $\delta > 1/2$ there exist B, C and β strictly positive such that for all $x > 0$ uniformly in x*

$$P\left(|T_m^c - \boldsymbol{E}[T_m^c]| + |L_m^c - \boldsymbol{E}[L_m^c]| \geq x m^{\delta} \right) \leq B e^{-xCm^{\beta}} \tag{12}$$

for large m.

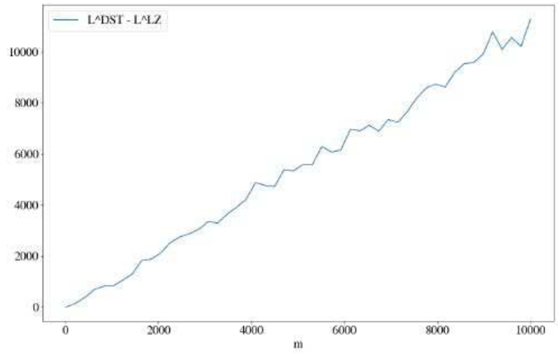

Figure 2 The difference $\mathbf{E}[L_m^c] - \mathbf{E}[\mathcal{L}_m^c]$ by simulation confirming that it grows linearly with m.

2.2 Results for the LZ78 Model

Let us start with the m-LZ model. For a given m, let $\mathcal{L}_m^c$ (note calligraphic $\mathcal{L}$) be the length of the LZ78 string composed of m phrases when the first phrase starts with symbol c. For memoryless sources, this quantity is equivalent to the path length L_m in the associated DST built over m independent strings. However, it is not the case for Markov sources. In Section 4 we prove Theorem 5 presented below by showing that $\mathbf{E}[L_m^c] - \mathbf{E}[\mathcal{L}_m^c] = \Theta(m)$, unlike in the memoryless case. Figure 2 compares the difference $\mathbf{E}[L_m^c] - \mathbf{E}[\mathcal{L}_m^c]$ obtained by simulation results confirming our theoretical findings.

▶ **Theorem 5.** *For m given, let $m^* := m^*(m)$ be the root of $x - x\tau(x) - (m-x)\tau(m-x)$.*

(i) *The average length $\boldsymbol{E}[\mathcal{L}_m^c]$ of the LZ-sequence consisting of the first m phrases is (for the aperiodic case)*

$$\boldsymbol{E}[\mathcal{L}_m^c] = m\log m/h + \mu(m^*)m^* + \mu(m-m^*)(m-m^*) + m(1 - H(m^*/m)/h) + O(m^\delta) \tag{13}$$

where $H(x) = -x\log x - (1-x)\log(1-x)$ is the binary entropy and h the source entropy.

(ii) *For all $\delta > 1/2$ there exist $B, C, \beta > 0$, and $\gamma > 0$ such that uniformly for all $x > 0$*

$$P\left(|\mathcal{L}_m^c - E[\mathcal{L}_m^c]| \geq xm^\delta\right) \leq Bm^\gamma e^{-xCm^\beta} \tag{14}$$

for large m.

▶ Remark. The property of function $\tau(\cdot)$ implies that the equation $x - x\tau(x) - (m-x)\tau(m-x)$ has a single root as we will see in the proof of Section 4. Notice that m^*/m converges to $\bar{\tau}$ in the aperiodic case, and similarly $\mu(m^*)m^* + \mu(m-m^*)(m-m^*)$ is asymptotically equivalent to $\bar{\mu}m$. In the periodic case there will be small periodic contributions (contained in $\tau(m)$ and $\mu(m)$) as shown in Theorem 3. Notice that $H(m^*/m)$ is the tail symbol entropy, which is equal to h when the source is memoryless.

Our next goal is to present large deviation for the number of LZ phrases in the n-LZ model. Let M_n^c be the number of phrases obtained by parsing a Markovian sequence of length n starting with symbol c. By the renewal equation (1) we have $P(M_n^c > m) = P(\mathcal{L}_m^c < n)$ for all legitimate m and n. This allows us to read large deviation of M_n^c from Theorem 5. Following the footsteps of Theorem 2 of [5] we arrive at our next main result.

▶ **Theorem 6.** *For all $\delta > 1/2$ there exist B, C, β, and γ all strictly positive such that*

$$P\left(|M_n^c - \ell_c^{-1}(n)| \geq xn^\delta\right) \leq Bn^\gamma e^{-xCn^\beta}$$

where $\ell_c^{-1}(.)$ is the inverse function of $\ell_c(m) = \ell(m) + o(1)$ defined as $\ell(m) = \frac{m}{h}(\log m + \beta(m))$ with

$$\beta(m) = h\mu(m^*)m^*/m + h\mu(m - m^*)(m - m^*)/m - h + H(m^*/m)$$

where m^* is defined in Theorem 5 and $\mu(m)$ has extra fluctuating function in the periodic case.

Using Theorem 6 we can find a precise estimate on the LZ78 redundancy. Indeed, a good approximation for the LZ78 code length is $C_n^c = M_n^c(\log M_n^c + 1)$. The average conditional redundancy is defined as $r_n^c := \mathbf{E}[C_n^c]/n - h$, while the total average redundancy is $r_n = \pi_a r_n^a + \pi_b r_n^b$.

▶ **Corollary 7.** *The average redundancy rate r_n satisfies for all $\frac{1}{2} < \delta < 1$:*

$$r_n = h\frac{1 - \beta(\ell^{-1}(n))}{\log \ell^{-1}(n) + \beta(\ell^{-1}(n))} + O(n^{\delta-1}\log n) \sim h\frac{1 - \beta(\ell^{-1}(n))}{\log n},$$

and more specifically in the aperiodic case we have

$$r_n \sim h\frac{1 - \bar{\mu}}{\log n} + \frac{H(\bar{\tau}) - h}{\log n}$$

where $m^*/m \to \bar{\tau}$.

3 Proof of Theorem 4 for DST

Now we prove Theorem 4, that is, the joint large deviations for T_m^c and L_m^c in the m-DST model. We use Chernoff's bounds, so we need to introduce some bivariate generating functions. Define $P_{m,k,\ell}^c = P(T_m^c = k \ \& \ L_m^c = \ell)$, $P_m^c(u, v) = \mathbf{E}[u^{T_m^c} v^{L_m^c}] = \sum_{k,\ell} P_{m,k,\ell}^c u^k v^\ell$ and $P_c(z, u, v)$ to be the Poisson generating function $P_c(z, u, v) = \sum_m P_n^c(u, v)\frac{z^m}{m!}e^{-z}$. The following partial differential equation for $P_c(z, u, v)$ is easy to establish from (5)

$$\partial_z P_c(z, u, v) + P_c(z, u, v) = (uP(a|c) + P(b|c))P_a(P(a|c)zv, u, v)P_b(P(b|c)zv, u, v).$$

Lemma below is equivalent to Theorem 10 of [5] so we skip the proof in this conference paper.

▶ **Lemma 8.** *For all reals $\varepsilon' > 0$ and $\epsilon > 0$, there exists $0 < \vartheta < \pi/2$ and a complex neighborhood $\mathcal{U}(0)$ of 0 such that iuniformly for $(t_1, t_2) \in \mathcal{U}(0)^2$ and $|\arg(z)| < \vartheta$ so that $\log(P_c(z, e^{t_1|z|^{-\varepsilon'}}, e^{t_2|z|^{-\varepsilon'}}))$ exists and $\log(P_c(z, e^{t_1|z|^{-\varepsilon'}}, e^{t_2|z|^{-\varepsilon'}}) = O(z^{1+\varepsilon})$.*

To prove Theorem 4 we need the following property that will be established in the final version of this paper.

▶ **Lemma 9.** *For all $\delta > 1/2$ there exists B such that*

$$\left|P_m^c(e^{\tau_1 m^{-\delta}}, e^{\tau_2 m^{-\delta}})\exp(-m^{-\delta}(\tau_1 \boldsymbol{E}[T_m^c] + \tau_2 \boldsymbol{E}[L_m^c]))\right| \leq B\sqrt{m}. \tag{15}$$

Now we proceed to prove Theorem 4. We apply Markov inequality for all θ and for all $x > 0$

$$P(|T_m^c - \mathbf{E}[T_m^c| + |L_m^c - \mathbf{E}[L_m^c]| \geq 2xm^\delta) \leq P(|T_m^c - \mathbf{E}[T_m^c]| \geq xm^\delta \vee (|L_m^c - \mathbf{E}[L_m^c]| \geq xm^\delta)$$

$$\leq \left(P_m^c(e^\theta, 1)e^{-E[T_m^c]\theta} + P_m^c(e^{-\theta}, 1)e^{E[T_m^c])\theta}\right) e^{-x\theta m^\delta}$$

$$+ \left(P_m^c(1, e^\theta)e^{-E[L_m^c]\theta} + P_m^c(1, e^{-\theta})e^{E[L_m^c])\theta}\right) e^{-x\theta m^\delta}.$$

To complete the proof we will use (15) of Lemma 9. If we take $\tau_1 = \pm C$ and $\tau_2 = 0$ (and reverse) for some $C > 0$ such that $(\tau_1, \tau_2) \in \mathcal{U}(0)^2$, and $\theta = Cm^{-\delta'}$ for some $\delta' < \delta$, then we find $e^{\theta m^\delta} = e^{-Cm^\beta}$ with $\beta = \delta - \delta' > 0$, and

$$P(|T_m^c - \mathbf{E}[T_m^c]| + |L_m^c - \mathbf{E}[L_m^c]| \geq 2xm^\delta) \leq 4\sqrt{m}Be^{-xCm^\beta}$$

which prove (12) of Theorem 4. We can readjust by taking $0 < \beta' < \beta$ and the value of B to omit the factor $\sqrt{m}$.

4 Proof of Theorem 5 for LZ

We now consider the LZ78 algorithm over a single infinite sequence generated by a Markov source, that is, the n-LZ model and connect it to the n-DST model in which the path length is equal to n (over a variable number of independently inserted strings). In the m-LZ model there are exactly m LZ phrases, each being a block carved in the Markovian sequence. The blocks are *not* i.i.d Markovian sequences.

Let $\mathcal{P}_{m,n}^c$ be the probability that the length of the first m LZ phrases is exactly n (when the first symbol is c), leading to the n-LZ model. Notice that not every pair (n, m) is feasible in the LZ model since by adding another phrase the path length may "jump" by more than one. We are interested in finding an asymptotic estimate of $\mathcal{P}_{m,n}^c$. We start by introducing yet another model. Let $\mathbf{s}$ be a sequence of m symbols, namely $\mathbf{s} = (c_1, \ldots, c_m) \in \mathcal{A}^m$. For $c \in \mathcal{A}$ we now compute the probability $\mathcal{P}_{\mathbf{s},n}^c$ that an infinite Markovian sequence starting with symbol c when parsed by LZ algorithm satisfies the following two properties: (i) the first m blocks have tail symbols $c_i \in \mathbf{s}$ for $i \leq m$ so that c_i is the first symbol of block $i+1$; (ii) the length of the first m LZ phrases is equal to n. If a string satisfies these two conditions, then we say it is $(\mathbf{s}, n)$ compatible and that it belongs to the $(\mathbf{s}, n)$-LZ model.

Given a string $\mathbf{s}$ of tail symbols we denote by $\mathbf{t}_c^a(\mathbf{s})$ (resp. $\mathbf{t}_c^b(\mathbf{s})$) the subsequence of $\mathbf{s}$ consisting of tail symbols of the LZ blocks starting with symbol a (resp. starting by symbol b). Now, it is easy to see that given the initial symbol c we can deduce the sequence of tails symbols and initial symbols of all phrases just by looking at the sequence $\mathbf{s}$, where the initial symbol of the next phrase is the tail symbol of the previous phrase. For example, if $\mathbf{s} = (a, b, a, b, b)$ and $c = a$ we have the following tail symbol and initial symbol sequence displayed in the following table:

block #	initial symbol	tail symbol
1	a	a
2	a	b
3	b	a
4	a	b
5	b	b

By taking the blocks (phrases) starting with $c = a$ we find $\mathbf{t}_a^a(\mathbf{s}) = (a, b, b)$ and the blocks starting with b yield $\mathbf{t}_a^b(\mathbf{s}) = (a, b)$.

Now we consider a sequence $\mathbf{t}$ of m symbols and introduce a new n-DST model which we call $(\mathbf{t}, n)$-DST model. We define by $P^c_{\mathbf{t},n}$ the probability that m i.i.d. (independent) Markovian sequences all starting with c satisfy the following two conditions (notice that we use roman P for this probability and calligraphic $\mathcal{P}$ for LZ model): (i) the tail symbol sequence follows the sequence $\mathbf{t}$; (ii) the external path length of the DST is exactly n. We will say that such m strings are $(\mathbf{t}, n)$-fit if they satisfy the above conditions and call it $(\mathbf{t}, n)$-DST model. We also define

$$P^c_{m,k,n} = \sum_{\mathbf{t}:\ |\mathbf{t}|=m, |\mathbf{t}|_a=k} P^c_{\mathbf{t},n} \tag{16}$$

with $|\mathbf{t}|$ being the length of sequence $\mathbf{t}$ and $|\mathbf{t}|_a$ being the number of symbols equal to a in it.

We finally establish the following fundamental lemma that connects the above two parameters which also connects the LZ parsing over a single Markovian sequence and the DST made of independent Markovian sequences, that is, $(\mathbf{s}, n)$-LZ model and $(\mathbf{t}, n)$-DST model where $\mathbf{t}$ is a function of $\mathbf{s}$.

▶ **Lemma 10.** *For any $\boldsymbol{s} \in \mathcal{A}^m$ we have*

$$\mathcal{P}^c_{\boldsymbol{s},n} = \sum_{n_a} P^a_{\boldsymbol{t}^a_c(\boldsymbol{s}),n_a} P^b_{\boldsymbol{t}^b_c(\boldsymbol{s}),n-n_a} \tag{17}$$

where n_c (equal either to n_a or n_b) is the path length in n_c-DST model with all strings starting with c, and $\boldsymbol{t}^a_c(\boldsymbol{s})$, $\boldsymbol{t}^b_c(\boldsymbol{s})$ are substrings of $\boldsymbol{s}$ as defined above.

Proof. In this conference paper, we give a proof using an example to ease the presentation. Let us consider $X = aabbababab\cdots$ which results in the following LZ blocks: $()(a)(ab)(b)(aba)(ba)(b\cdots)$. Or equivalently $X = \mathbf{aa}b\mathbf{ba}ba\mathbf{b}a\mathbf{b}\cdots$ where the initial block (phrase) symbols are displayed in bold. We notice that the first five blocks (excluding the initial empty block) accounts for a string of length 9. Thus the sequence X is $(\mathbf{s}, 9)$ compatible with $\mathbf{s} = (a, b, a, b, b)$. Given that X starts with symbol a we have $P(X) = P(\mathbf{a}|a)P(a\mathbf{a}|a)P(ab\mathbf{b}|a)P(b\mathbf{a}|b))P(aba\mathbf{b}|a)P(ba\mathbf{b}|b)$. Notice that we display in bold the tail symbol of each block (which is the initial symbol of the next block). We must incorporate $P(X)$ into $P^a_{\mathbf{s},9}$. In fact X should be viewed as the set of (infinite) strings having $aabbababab$ as the common prefix. We can rewrite $P(X)$ by regrouping the terms with respect to the initial symbol of each block as: $P(X) = [P(aa|a)P(abb|a)P(abab|a)] \times [P(ba|b)P(bab|b)]$. Observe that the sequence of strings $(aa, abb, abab)$ are the prefixes of a set of tuples of independent infinite strings that are all $(\mathbf{s}^a, 6)$ compatible with $\mathbf{s}^a = \mathbf{t}^a_a(\mathbf{s}) = (a, b, b)$ under the condition that the strings start with symbol a (the path length in the DST excludes the tail symbols, thus we must remove one from the length of each prefix). The probability of such event is exactly $P(aa|a)P(abb|a)P(abab|a)$ and must be incorporated in $P^a_{\mathbf{s}^a,6}$. Furthermore, these sequences are used to build one (left) part of the DST tree with independent Markov strings all starting with a. The same holds for the sequence of strings (ba, bab) which is $(\mathbf{s}^b, 3)$ compatible with $\mathbf{s}^b = \mathbf{t}^b_a(\mathbf{s}) = (a, b)$ and used to build the other part (right) of the DST tree. This leads to (17). ◀

The next crucial lemma connects n-LZ and n-DST models.

▶ **Lemma 11.** *The following holds*

$$\begin{aligned}\mathcal{P}^c_{m,n} \;\leq\; & \sum_{n_a}\sum_{k}\sum_{m_a} \big(P^a_{m_a,k,n_a} P^b_{m-m_a,m_a-k,n-n_a} \\ & + P^a_{m_a,k,n_a} P^b_{m-m_a,m_a-k-1,n-n_a} + P^a_{m_a,k,n_a} P^b_{m-m_a,m_a-k+1,n-n_a}\big)\end{aligned} \tag{18}$$

where n_a is the total path length of the first m_a phrases starting with an "a".

Proof. We naturally have $\mathcal{P}^c_{m,n} = \sum_{|\mathbf{s}|=m} \mathcal{P}^c_{\mathbf{s},n}$ where $|\mathbf{s}|$ is the length of the sequence $\mathbf{s}$. Similarly we have $P^c_{m,k,n} = \sum_{\mathbf{t},|\mathbf{t}|=m,|\mathbf{t}|_a=k} P^c_{\mathbf{t},n}$ with $|\mathbf{t}|_a$ is the number of symbols identical to a in $\mathbf{t}$. The rest follows from Lemma 10 but we need to take into account some boundary effects.

Let's look at it in more details. By (17) and above we find

$$\mathcal{P}^c_{m,n} = \sum_{|\mathbf{s}|=m} \sum_{n_a} P^a_{\mathbf{t}^a_c(\mathbf{s}),n_a} P^b_{\mathbf{t}^b_c(\mathbf{s}),n-n_a}.$$

We now partition $\mathcal{A}^m$into four sets $\mathcal{S}^c_0(m)$, $\mathcal{S}^c_1(m)$, $\mathcal{S}^c_2(m)$ and $\mathcal{S}^c_3(m)$:

- $\mathbf{s} \in \mathcal{S}^c_0(m)$: if neither of the initial symbol c or the final symbol of $\mathbf{s}$, namely c_m is identical to a. Thus the total number of tail symbols equal to a, namely $|\mathbf{s}|_a$ is equal to $|\mathbf{t}^a_c(\mathbf{s})|$.
- $\mathbf{s} \in \mathcal{S}^c_1(m)$: if both the final symbol and c are equal to a so that the total number of tail (and initial) symbols equal to a is $|\mathbf{t}^a_c(\mathbf{s})|$.
- $\mathbf{s} \in \mathcal{S}^c_2(m)$: if $c = a$ but $c_m \neq a$ so that the number of tail symbols equal to a is $|\mathbf{t}^a_c(\mathbf{s})| - 1$.
- $\mathbf{s} \in \mathcal{S}^c_3(m)$: if $c \neq a$ but the final symbol $c_m = a$. Thus the number of tail symbols equal to a is $|\mathbf{t}^a_c(\mathbf{s})| + 1$.

Regrouping we have

$$\mathcal{P}^c_{m,n} = \sum_{\mathbf{s}\in\mathcal{S}^c_0(m)\cup\mathcal{S}^c_1(m)} \mathcal{P}^c_{\mathbf{s},n} + \sum_{\mathbf{s}\in\mathcal{S}_2(m)} \mathcal{P}^c_{\mathbf{s},n} + \sum_{\mathbf{s}\in\mathcal{S}_3(m)} \mathcal{P}^c_{\mathbf{s},n}.$$

Now we have to deal with the right hand side of (18), that is, with the DST model. Let $\mathcal{T}_1(m)$ be the set of pairs of *arbitrary* sequences denoted as $(\mathbf{t}^a, \mathbf{t}^b)$ such that $|\mathbf{t}^a| + |\mathbf{t}^b| = m$ and $|\mathbf{t}^a|_a + |\mathbf{t}^b|_a = |\mathbf{t}^a|$. We notice that for $\mathbf{s} \in \mathcal{S}^c_1(m) \cup \mathcal{S}^c_2(m)$: $(\mathbf{t}^a_c(\mathbf{s}), \mathbf{t}^b_c(\mathbf{s})) \in \mathcal{T}_1(m)$, hence

$$\begin{aligned}\sum_{\mathbf{s}\in\mathcal{S}^c_0(m)\cup\mathcal{S}^c_1(m)} \mathcal{P}^c_{\mathbf{s},n} &= \sum_{n_a} \sum_{\mathbf{s}\in\mathcal{S}^c_0\cup\mathcal{S}^c_1(m)} P^a_{\mathbf{t}^a(\mathbf{s}),n_a} P^b_{\mathbf{t}^b(\mathbf{s}),n-n_a}\\ &\leq \sum_{n_a} \sum_{(\mathbf{t}_a,\mathbf{t}_b)\in\mathcal{T}_1(m)} P^a_{\mathbf{t}^a,n_a} P^b_{\mathbf{t}^b,n-n_a}.\end{aligned}$$

Notice that we have an upper bound, since for some pair $(\mathbf{t}^a, \mathbf{t}^b)$ in $\mathcal{T}^c_1(m)$ there may not exist $\mathbf{s} \in \mathcal{S}^c_1(m) \cup \mathcal{S}^c_2(m)$ such that $\mathbf{t}^a = \mathbf{t}^a(\mathbf{s})$ and $\mathbf{t}^b = \mathbf{t}^b(\mathbf{s})$. For example, let $c = a$ and for $m = 4$ we set $\mathbf{t}^a = (a, b)$ and $\mathbf{t}^b = (b, a)$, so that $|\mathbf{t}^a|_a + |\mathbf{t}^b|_a = |\mathbf{t}^a|$ but it is impossible to find $\mathbf{s}$ such that $(\mathbf{t}^a_a(\mathbf{s}), \mathbf{t}^b(\mathbf{s})) = (\mathbf{t}^a, \mathbf{t}^b)$.

Thanks to (16) we have $\sum_{\mathbf{t}:\ |\mathbf{t}|=m,|\mathbf{t}|_a=k} P^c_{\mathbf{t},n} = P^c_{m,k,n}$ leading to

$$\sum_{(\mathbf{t}_a,\mathbf{t}_b)\in\mathcal{T}_1(m)} \sum_{n_a} P^a_{\mathbf{t}^a,n_a} P^b_{\mathbf{t}^b,n-n_a} = \sum_{m_a,k} P^a_{m_a,k,n_a} P^b_{m-m_a,m_a-k,n-n_a}.$$

This proves the first term in the right hand side of (18). To prove the other two terms we introduce $\mathcal{T}_2(m)$ as the set of pairs of sequence $(\mathbf{t}^a, \mathbf{t}^b)$ such that $|\mathbf{t}^a| + |\mathbf{t}^b| = m$ and $|\mathbf{t}^a|_a + |\mathbf{t}^b|_a = |\mathbf{t}^a| - 1$. In this case

$$\sum_{\mathbf{s}\in\mathcal{S}_2(m)} \mathcal{P}^c_{\mathbf{s},n} \leq \sum_{n_a} \sum_{(\mathbf{t}^a,\mathbf{t}^b)\in\mathcal{T}_2(m)} P^a_{\mathbf{t}^a,n_a} P^b_{\mathbf{t}^b,n-n_a},$$

and the second term of (18) is proved. And finally with $\mathcal{T}_3(m)$ as the set of pairs of sequence $(\mathbf{t}^a, \mathbf{t}^b)$ such that $|\mathbf{t}^a| + |\mathbf{t}^b| = m$ and $|\mathbf{t}^a|_a + |\mathbf{t}^b|_a = |\mathbf{t}^a| + 1$, we establish the third term of (18). ◀

To finish the proof of Theorem 5 we now use the previous lemmas to upper bound $\mathcal{P}^c_{m,n}$. Let $\mathcal{P}^c_{m,n} \le K^c_{m,n}(0) + K^c_{m,n}(1) + K^c_{m,n}(-1)$ with

$$K^c_{m,n}(i) = \sum_{m_a}\sum_{n_a}\sum_{k} P^a_{m_a,k,n_a} P^b_{m-m_a,m_a-k-i,n-n_a}.$$

To simplify our presentation we only study $K^c_{m,n}(0)$. First, we rewrite the bound in Theorem 4 for the DST model as follows: for $\delta > 1/2$ there exist B and C strictly positive such that

$$P^c_{m,k,n} \le B \exp\left[-Cm^{-\delta}|k - \mathbf{E}[T^c_m]| - Cm^{-\delta}|n - \mathbf{E}[L^c_m]|\right].$$

Thus

$$K^c_{m,n}(0) \le \textstyle\sum_{m_a+m_b=m}\sum_{k\le m_a}\sum_{n_a+n_b=n} B^2 \exp\left[-Cm_a^{-\delta}|k - \mathbf{E}[T^c_{m_a}]\right.$$
$$\left.-Cm_a^{-\delta}|n_a - \mathbf{E}[L^a_{m_a}| - Cm_b^{-\delta}|m_a - k - \mathbf{E}[T^b_{m_b}] - Cm_b^{-\delta}|n_b - \mathbf{E}[L^b_{m_b}|\right].$$

From here we use $m_a, m_b \le m$ to find

$$Cm_a^{-\delta}|k - \mathbf{E}[T^c_{m_a}] + Cm_a^{-\delta}|n_a - \mathbf{E}[L^a_{m_a}| + Cm_b^{-\delta}|m_a - k - \mathbf{E}[T^b_{m_b}] + Cm_b^{-\delta}|n_b - \mathbf{E}[L^b_{m_b}| \ge$$
$$Cm^{-\delta}|k - \mathbf{E}[T^c_{m_a}] + Cm^{-\delta}|n_a - \mathbf{E}[L^a_{m_a}| + Cm^{-\delta}|m_a - k - \mathbf{E}[T^b_{m_b}] + Cm^{-\delta}|n_b - \mathbf{E}[L^b_{m_b}|$$
$$\ge Cm^{-\delta}|m_a - \mathbf{E}[T^a_{m_a}] - \mathbf{E}[T^b_{m_b}]| + Cm^{-\delta}|n - \mathbf{E}[L^a_{m_a}] - \mathbf{E}[L^b_{m_b}]|.$$

Replacing the $\mathbf{E}[T^c_m]$ by $\tau_c(m)m$ and $\mathbf{E}[L^c_m]$ by $m\log m/h + m + m\mu_c(m)$ we arrive at

$$K^c_{m,n}(0) \le B^2 m \sum_{m_a+m_b=m} \exp\left(-Cm^{-\delta}|m_a - m_a\tau_a(m_a) - m_b\tau_b(m_b)|\right)$$
$$\times \exp\left(-Cm^{-\delta}|n - m\log m/h + m(H(m_a/m)/h - 1) - m_a\mu_a(m_a) - m_b\mu_b(m_a)|\right).$$

Without changing the order of magnitude we further can replace $\tau_c(m)$ by $\tau(m)$ and $\mu_c(m)$ by $\mu(m)$.

We now focus only on the aperiodic case and set $\tau(m) = \bar{\tau}m$ and $\mu(m) = \bar{\mu}m$. (We know that even in this case for small values of m, the $\mu(m)$ and $\tau(m)$ are not exactly linear in m, but we handle it later.) Thus our term $K^c_{m,n}(0)$ is bounded by

$$B^2 m \sum_{m_a \le m} \exp[-Cm^{-\delta}|m_a - \bar{\tau}m|] \exp[-Cm^{-\delta}|n - m\log m/h - \bar{\mu}m + m(H(m_a/m)/h - 1)|].$$

If we take any $\delta' > \delta$ we find

$$K^c_{m,n}(0) \le B^2 m \sum_{m_a \le m} \exp[-Cm^{-\delta}|m_a - \bar{\tau}m|]$$
$$\times \exp[-Cm^{-\delta'}|n - m\log m/h - \bar{\mu}m + m(H(m_a/m)/h - 1)|].$$

We observe that $\exp[-Cm^{-\delta}|m_a - \bar{\tau}m|]$ attains its maximum at $m_a = m^* = \bar{\tau}m$. Thus

$$K^c_{m,n}(0) \le B^2 \sum_{m_a \le m^*} e^{Cm^{-\delta}(m-m^*)} \times \exp[-Cm^{-\delta'}|n - m\log m/h - \bar{\mu}m + m(H(m_a/m)/h - 1)|]]$$
$$+B^2 \sum_{m_a \ge m^*} e^{Cm^{-\delta}(m^*-m)} \times \exp[-Cm^{-\delta'}|n - m\log m/h - \bar{\mu}m + m(H(m_a/m)/h - 1)|]].$$

Notice that the terms $e^{Cm^{-\delta}(m-m^*)}$ and $e^{Cm^{-\delta}(m^*-m)}$ form a geometrically decreasing series with rate $e^{-Cm^{-\delta}}$. Since $|mH((m_a+1)/m) - mH(m_a/m)| \leq \log m$, the term

$$\exp[-Cm^{-\delta'}|n - m\log n/h - \bar{\mu}m + m(H(m_a/m)/h - 1)|]]$$

is at most geometrically increasing with a rate $e^{m^{-\delta'}\log m/h}$ which is smaller than $e^{Cm^{-\delta}}$. Therefore, the whole series has its maximum at $m_a = m^*$ and

$$K^c_{m,n}(0) \leq 2B^2 \sum_{k=0^\infty} e^{-Ck(m^{-\delta} - \log m/hm^{-\delta'})}$$

$$\times \exp[-Cm^{-\delta'}|n - m\log n/h - \bar{\mu}m + m(H(m^*/m)/h - 1)|]]$$

$$= \frac{2B^2}{1 - e^{-(m^{-\delta} - \log m/hm^{-\delta'})C}}$$

$$\times \exp[-Cm^{-\delta'}|n - m\log m/h - \bar{\mu}m + m(H(m^*/m)/h - 1)|]]$$

$$= O(2B^2m^\delta)\exp[-Cm^{-\delta'}|n - m\log m/h - \bar{\mu}m + m(H(\bar{\tau})/h - 1)|]].$$

Including all contributions, the final estimate for some $B' > 0$ is

$$\mathcal{P}^c_{m,n} \leq B'm^{1+\delta}\exp[-Cm^{-\delta}|n - m\log m - \bar{\mu}m + m(H(\bar{\tau})/h - 1)|].$$

This gives the large deviation estimate and $\mathbf{E}[\mathcal{L}^c_{m,n}] = m\log m/h + \bar{\mu}m - m(H(\bar{\tau})/h - 1) + O(m^\delta)$ by Fact 1. We recognize in $H(\bar{\tau})$ the entropy of the tail symbol.

In fact the quantities $\tau(m)$ and $\mu(m)$ are not exactly $\bar{\tau}m$ and $m\bar{\mu}$. To handle it we observe that due to their slowly varying properties, the function $\exp(-Cm^{-\delta}|m_a - \tau(m_a)m_a - \tau(m - m_b)(m - m_a)|$ attains the maximum for m^* such that

$$m^* = -\tau_a(m^*)m^* - \tau_b(m^*)(m - m^*).$$

Indeed the function $m_a - \mathbf{E}[T^a_{m_a}] - \mathbf{E}[T^b_{m_b}]$ is strictly increasing thus this value is unique. Then again $\mathbf{E}[\mathcal{L}^c_m] = m\log m/h + m^*\mu(m^*) + (m - m^*)\mu(m - m^*) - m(H(m^*/m)/h - 1)$, and therefore $\mathbf{E}[L^c_m] + mH(m^*/m) + o(m)$. The latter is equal to $\mathbf{E}[L^c_m] + mH(\bar{\tau}) + o(m)$ in the aperiodic case. To complete the proof of Theorem 5 we just use Fact 1 applied to $\mathcal{L}_m$.

5 Conclusions

In this paper we analyze the Lempel-Ziv'78 algorithm for binary Markov sources, a problem left open since the algorithm inception. To handle the strong dependency between Markov phrases, we introduce and precisely analyze the so called tail symbol which is the first symbol of the next phrase in the LZ78 parsing. We focus here on the large deviations for the number of phrases in the LZ78 and also give a precise asymptotic expression for the redundancy which is the excess of LZ78 code over the entropy of the source. In future work we plan to extend our analysis to non-binary Markov sources and present some bounds on the central limit theorem. Furthermore, we shall study LZ78 for Markov sources of higher order, however, this will require a new approach to the tail symbols which may span over consecutive phrases.

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A Proof of Theorem 3(i): Mean

We first analyze asymptotically $\mathbf{X}(z) = (X_a(z), X_b(z))$ that satisfies the system of differential-functional equations (6). We solve this system, and then apply Mellin transform and depoissonization to prove Theorem 3(i).

Since for all integer m, we have $T_m^c \leq m$, we notice that the function $X_c(z)$ is $O(z)$ both when $z \to \infty$ and when $z \to 0$. Thus the function $\mathbf{X}(z)$ has no Mellin transform defined as $X_c(s) = \int_0^\infty X_c(z) z^{s-1} dz$ (see [15] for more on the Mellin transform). To correct this we introduce $\tilde{X}_c(z) = X_c(z) - G_c(z)$ with $G_c(z) = (\mathbf{E}[T_1^c]z + \mathbf{E}[T_2^c]z^2/2)e^{-z}$ which is $O(z^3)$ when $z \to 0$, where $\mathbf{E}[T_1^c]$ and $\mathbf{E}[T_2^c]$ are defined in (7).

The Mellin transform $X_c^*(s)$ of $\tilde{X}_c(z)$ on the strip $\Re(s) \in]-3, -1[$ exists. The Mellin transform of $\partial_z \tilde{X}_c(z)$ exists too on the strip $\Re(s) \in]-2, 0[$. Thus the two Mellin transforms coexist on the strip $\Re(s) \in]-2, -1[$ and satisfies [15]

$$- (s-1)(X_c^*(s-1) + G_c^*(s)) + X_c^*(s) + G_c^*(s)$$
$$= P(a|c)^{-s}(X_a^*(s) + G_a^*(s)) + P(b|c)^{-s}(X_b^*(s) + G_b^*(s))$$

where $G_c^*(s)$ for $c \in \mathcal{A}$ is the Mellin transform of $G_c(z)$ and has the explicit expression $\mathbf{E}[T_1^c]\Gamma(1+s) + \mathbf{E}[T_2^c]\Gamma(s+2)/2$. This expression is here for completeness.

An alternative but convenient way to see this equations is to consider the vector $\mathbf{X}^*(s)$ made of the quantities $X_c^*(s)$, $c \in \mathcal{A}$ which is also the Mellin transform of the vector $\tilde{\mathbf{X}}(z)$ made of the coefficients $\tilde{X}_c(z)$. This yields the linear equation

$$-(s-1)(\mathbf{X}^*(s-1) + \mathbf{G}^*(s-1)) + \mathbf{X}^*(s) + \mathbf{G}^*(s) =$$

$$= \mathbf{P}(s)(\mathbf{X}^*(s) + \mathbf{G}^*(s))$$

where $\mathbf{G}^*(s)$ is the vector of the $G_c^*(s)$. It can be rewritten in

$$(s-1)(\mathbf{X}^*(s-1) + \mathbf{G}^*(s-1)) = (\mathbf{I} - \mathbf{P}(s))(\mathbf{X}^*(s) + \mathbf{G}^*(s)).$$

This kind of equation has been studied in [7] where we introduce a new function $\mathbf{x}(s)$

$$\mathbf{X}^*(s) + \mathbf{G}^*(s) = \Gamma(s)\mathbf{x}(s).$$

Thus the equation becomes $\mathbf{x}(s-1) = (\mathbf{I} - \mathbf{P}(s))\mathbf{x}(s)$, which leads to $\mathbf{x}(s) = \prod_{i\geq 0}(\mathbf{I} - \mathbf{P}(s-i))^{-1}\mathbf{K}$ where $\mathbf{K}$ is a constant vector. Notice that the matrices very likely don't commute thus the product order is specified from the left to right. Indeed we have

$$\mathbf{K} = \left(\prod_{j\geq 2}(\mathbf{I} - \mathbf{P}(-j))^{-1}\right)^{-1} \mathbf{x}(-2) = \prod_{j=-\infty}^{j=2}(\mathbf{I} - \mathbf{P}(j))\mathbf{x}(-2). \tag{A.1}$$

To handle it we need an explicit formula for $\mathbf{x}(-2)$. The following lemma from [7] is useful in this regard. We provide a proof for completeness.

▶ **Lemma 12.** *Let $\{f_n\}_{n=0}^{\infty}$ be a sequence of real numbers having the Poisson transform*

$$\widetilde{F}(z) = \sum_{n=0}^{\infty} \tilde{f}_n \frac{z^n}{n!} e^{-z} := \sum_{n=0}^{\infty} f_n \frac{z^n}{n!}, \tag{A.2}$$

which is an entire function. Furthermore, let its Mellin transform $F(s)$ have the following factorization

$$F(s) = \mathcal{M}[\widetilde{F}(z); s] = \Gamma(s)\gamma(s).$$

Assume that $F(s)$ exists for $\Re(s) \in (-2,-1)$, and that $\gamma(s)$ is analytic for $\Re(s) \in (-\infty,-1)$. Then

$$\gamma(-n) = \sum_{k=0}^{n} \binom{n}{k} (-1)^k \tilde{f}_k = (-1)^n f_n, \quad \text{for} \quad n \geq 2. \tag{A.3}$$

Proof. Notice that f_n and $\tilde{f}_n$ are related by [15]

$$\tilde{f}_n = \sum_{k=0}^{n} \binom{n}{k} (-1)^{n-k} f_k \ , \qquad n \geq 0 \ .$$

Define for some fixed $M \geq 2$, the function $\widetilde{F}_M(z) = \sum_{n=0}^{M-1} f_n \frac{z^n}{n!}$. Due to our assumptions, we can continue $F(s)$ analytically to the whole complex plane except $s = -2, -3, \ldots$. In particular, for $\Re(s) \in (-M, -M+1)$ we have $F(s) = \mathcal{M}[\widetilde{F}(z) - \widetilde{F}_M(z); s]$. As $s \to -M$, due to the factorization $F(s) = \Gamma(s)\gamma(s)$, we have

$$F(s) = \frac{1}{s+M} \frac{(-1)^M}{M!} \gamma(-M) + O(1) \ ;$$

thus by the inverse Mellin transform, we have

$$\widetilde{F}(z) - \widetilde{F}_M(z) = \frac{(-1)^M}{M!} \gamma(-M) z^M + O(z^{M+1}) \quad \text{as} \quad z \to 0 \ . \tag{A.4}$$

But

$$\widetilde{F}(z) - \widetilde{F}_M(z) = \sum_{i=M}^{\infty} f_n \frac{z^n}{n!} = f_M \frac{z^M}{M!} + O(z^{M+1}) \ . \tag{A.5}$$

Comparing (A.4) and (A.5) shows that $\gamma(-M) = (-1)^M f_M = \sum_{k=0}^{M} \binom{M}{k} (-1)^k \tilde{f}_k$. ◀

Now we can compute $\mathbf{x}(-2)$ using above and (7) leading to

$$\mathbf{x}(-2) = \begin{bmatrix} T_2^a - 2P(a|a) \\ T_2^b - 2P(a|b) \end{bmatrix}. \tag{A.6}$$

In another notation $\mathbf{x}(-2) = (\mathbf{P}^2 - \mathbf{P})\mathbf{e}_a$, where $\mathbf{e}_a$ is the vector made of a single 1 at a position and zero otherwise.

Next, we notice that the vector

$$\Gamma(s) \prod_{i \geq 0} (\mathbf{I} - \mathbf{P}(s-i))^{-1} \prod_{j=-\infty}^{j=-2} (\mathbf{I} - \mathbf{P}(j)) \mathbf{x}(-2)$$

may have a double pole on $s = -1$ since $\Gamma(s)$ has a pole and also $(\mathbf{I} - \mathbf{P}(s))^{-1}$ since $\mathbf{I} - \mathbf{P}(-1) = \mathbf{I} - \mathbf{P}$ is singular. But in fact the pole multiplicity is reduced by one, as prove below. Let us also define

$$\mathbf{Q}(s) = \prod_{i \geq 1} (\mathbf{I} - \mathbf{P}(s-i))^{-1} \prod_{j=-\infty}^{j=-2} (\mathbf{I} - \mathbf{P}(j)).$$

Then $\mathbf{x}(s) = (\mathbf{I} - \mathbf{P}(s))^{-1} \mathbf{Q}(s) \mathbf{x}(-2)$.

We notice that when $s \to -1$, then $\mathbf{Q}(s) = \mathbf{I} + (s+1)\mathbf{Q}'(-1) + O((s+1)^2)$. Furthermore let $\lambda(s)$ be the main eigenvalue of matrix $\mathbf{P}(s)$ and $\mathbf{1}(s)$ and $\boldsymbol{\pi}(s)$ be respectively the right and left main eigenvectors. We have $\lambda(-1) = 1$, $\mathbf{1}(-1) = \mathbf{1}$ is all made of one's, and $\boldsymbol{\pi}(-1)$ is the stationary distribution of the Markov source.

From the matrix spectral representation [15] we have

$$\mathbf{P}(s) = \lambda(s) \mathbf{1}(s) \otimes \boldsymbol{\pi}(s) + \mathbf{R}(s) = \lambda(s) \boldsymbol{\Pi}(s) + \mathbf{R}(s) \tag{A.7}$$

where $\mathbf{R}(s)$ is the automorphism of the eigenplan orthogonal to the main eigenvector and $\boldsymbol{\Pi}(s) = \mathbf{1}(s) \otimes \boldsymbol{\pi}(s)$ where $\otimes$ is the tensor product. Note that $\boldsymbol{\Pi} \cdot \mathbf{P} = \mathbf{P} \cdot \boldsymbol{\Pi} = \boldsymbol{\Pi}$. Then

$$\begin{aligned} (\mathbf{I} - \mathbf{P}(s))^{-1} \quad &= \quad \frac{1}{1 - \lambda(s)} \mathbf{1}(-s) \otimes \boldsymbol{\pi}(s) \\ &\quad - \frac{1}{\lambda'(-1)} \left(\mathbf{1}'(-1) \otimes \boldsymbol{\pi}(-1) + \mathbf{1} \otimes \boldsymbol{\pi}'(-1) \right) + \mathbf{R}(-1)^{-1} + O(s+1). \end{aligned}$$

Finally

$$(\mathbf{I}-\mathbf{P}(s))^{-1}\mathbf{Q}(s)\mathbf{x}(-2) = \frac{\mathbf{1}\otimes\boldsymbol{\pi}(s)(\mathbf{I}-\mathbf{P})\mathbf{e}_a}{1-\lambda(s)} - \frac{1}{\lambda'(-1)}\left(\mathbf{1}'(-1)\otimes\boldsymbol{\pi}+\mathbf{1}\otimes\boldsymbol{\pi}'(-1)\right) + \mathbf{R}^{-1}(-1) + \frac{(s+1)}{1-\lambda(s)}\mathbf{1}\otimes\mathbf{Q}'(-1) + O(s+1).$$

Since

$$\frac{s+1}{1-\lambda(s)} \to -\frac{1}{\lambda'(-1)}$$

when $s\to -1$, and $\mathbf{\Pi}\mathbf{P}(\mathbf{I}-\mathbf{P})\mathbf{e}_a = (\mathbf{\Pi}-\mathbf{\Pi})\mathbf{e}_a = 0$. Also

$$\mathbf{R}^{-1}(-1)(\mathbf{I}-\mathbf{P})\mathbf{P}\mathbf{e}_a = \mathbf{P}\mathbf{e}_a - \langle\boldsymbol{\pi}\mathbf{P}\mathbf{e}_a\rangle\mathbf{1} = \mathbf{P}\mathbf{e}_a - \langle\boldsymbol{\pi}\mathbf{e}_a\rangle\mathbf{1}. \tag{A.8}$$

We finally have

$$\lim_{s\to -1}\mathbf{x}(s) = \mathbf{P}\mathbf{e}_a - \pi_a\mathbf{1} - \frac{1}{\lambda'(-1)}\mathbf{1}\langle\left(\boldsymbol{\pi}'(-1)+\boldsymbol{\pi}\mathbf{Q}'(-1)\right)(\mathbf{I}-\mathbf{P})\mathbf{P}\mathbf{e}_a\rangle, \tag{A.9}$$

where π_a is the coefficient of the stationary distribution $\boldsymbol{\pi}$ at symbol a.

Now we are in position to establish asymptotics of $X_c(z)$ for large z and through depoissonization asymptotics of $\mathbf{E}[T_m^c]$. The inverse Mellin transform is

$$\tilde{X}_c(z) = \frac{1}{2i\pi}\int_{x-i\infty}^{x+i\infty} X_c^*(s)z^{-s}ds \tag{A.10}$$

valid for all $x\in]-2,-1[$. Remembering that $T_c(z) = \tilde{X}_c(z) + P(a|c)z$ we have indeed

$$\tilde{\mathbf{X}}(z) = \frac{1}{2i\pi}\int_{x-i\infty}^{x+i\infty}\Gamma(s)\mathbf{x}(s)z^{-s}ds - \frac{1}{2i\pi}\int_{x-i\infty}^{x+i\infty}\mathbf{G}^*(s)z^{-s}ds. \tag{A.11}$$

We know that $\mathbf{T}(z)-\tilde{\mathbf{X}}(z)$ is decaying exponentially fast when $z\to\infty$.

Moving the line of integration toward the right, we meet a single pole at $s=-1$ of $\mathbf{G}^*(s)z^{-z}$ and its residues is $-z\mathbf{P}\mathbf{e}_a$. Then

$$\frac{1}{2i\pi}\int_{x-i\infty}^{x+i\inf ty}\mathbf{G}^*(s)z^{-s}ds = -\mathbf{P}\mathbf{e}_a + O(z^{-M})$$

for all $M>0$.

The value -1 is also a simple pole for $z^{-s}\Gamma(s)\mathbf{x}(s)$. We know that its residue is

$$-z\left(\mathbf{P}\mathbf{e}_a - \pi_a\mathbf{1} - \frac{1}{\lambda'(-1)}\mathbf{1}\langle\left(\boldsymbol{\pi}'(-1)+\boldsymbol{\pi}\mathbf{Q}'(-1)\right)(\mathbf{I}-\mathbf{P})\mathbf{P}\mathbf{e}_a\rangle\right). \tag{A.12}$$

Therefore we have

$$\mathbf{X}(z) = z\left(\pi_a + \frac{1}{\lambda'(-1)}\mathbf{1}\langle\left(\boldsymbol{\pi}'(-1)+\boldsymbol{\pi}\mathbf{Q}'(-1)\right)(\mathbf{I}-\mathbf{P})\mathbf{P}\mathbf{e}_a\rangle\right)\mathbf{1} + o(z). \tag{A.13}$$

For irrational case, we know that $s=-1$ is the only pole on the line $\Re(s)=-1$, leading to the error term $o(z)$ coming from other poles of $(\mathbf{I}-\mathbf{P}(s))^{-1}$ which may occur on the right half plan of $s=-1$.

But in the rational case, there is the possibility of other poles regularly spaced on the axis $\Re(s)=-1$ with some specific matrices $\mathbf{P}$ detailed in [7] where the coefficients α_{abc} are introduced. In these very specific cases (the uniform probability distribution on $\mathcal{A}$ is one of them) the $o(z)$ term should be replaced by a term $zQ_c(\log z)+O(z^{1-\epsilon})$, where Q_c is a periodic vector of very small amplitude and mean zero, and $\epsilon>0$ depends on the matrix $\mathbf{P}$. This proves Theorem 3(i).

B Proof of Theorem 3(ii): Variance

We now analyze asymptotically $\mathbf{V}(z) = (V_a(z), V_b(z))$ that satisfies the system of differential-functional equations (8). In order to apply depoissonization, for $\theta \in [0, \pi/2]$ we define $\mathcal{C}(\theta)$ as the complex cone containing the complex number z such that $|\arg(z)| \leq \theta$ on increasing domains [15, 5]

$$\mathcal{C}_k(\theta) = \{z, z \in \mathcal{C}(\theta) \& |z| \leq \rho^k\}$$

with $\rho = \min_c\{\frac{1}{P(a|c)}, \frac{1}{P(b|c)}\}$.

Our first goal is to prove that $V_c(z) = O(z)$. We shall use use the increasing domain approach [15] applied to (8) following the footsteps of the proof of Lemma 7A of [3]. From Fact 1 of [3] we conclude that

$$V_c(z) = V_c(\rho z)e^{-z(1-\rho)} + e^{-z}\int_{\rho z}^{z} e^x \left(V_a(P(a|c)x) + V_b(P(b|c)x) + g(x)\right) dx \tag{B.14}$$

where $g(z) = P(a|c) - P^2(a|c) + [X_z^c(z)]^2 = O(1)$. Indeed, it follows from Fact 1 of [3] that the differential equation like

$$f'(z) = b(z) - a(z)f(z) \tag{B.15}$$

satisfies

$$f(z) = f(z_0)e^{A(z_0)-A(z)} + \int_{z_0}^{z} b(x)e^{A(x)-A(z)}dx$$

where $A(z) = \int a(z)$ is the primitive function of $a(z)$. Setting in (B.15) $f(z) = V_c(z)$, $b(z) = V_a(P(a|c)z) + V_b(P(b|c)z) + g(z)$ and $a(z) = 1$ we obtain (B.14).

Now we apply induction over the increasing domains. In short, we assume that for $z \in \mathcal{C}_k(\theta)$ we have $|V_c(z)| \leq B_k|z|$ for some B_k. Using the induction of the increasing domains we prove, as in the Appendix of [3] that B_k are bounded. This completes the proof, after applying the depoissonization lemma of [4].

In order to find a precise estimate of the asymptotic development of $\mathbf{V}(z)$ we denote $\mathbf{V}^*(s)$ the Mellin transform of $\mathbf{V}(z)$. From (8) we arrive at

$$-(s-1)\mathbf{V}^*(s-1) + \mathbf{V}^*(s) = \mathbf{P}(s)\mathbf{V}^*(s) + \mathbf{g}^*(s),$$

where $\mathbf{g}^*(s)$ is the Mellin transform of the vector made of the coefficients $(\partial_z X_c(z))^2$. Let $\mathbf{V}^*(s) = \Gamma(s)\mathbf{B}(s)$ and $\mathbf{g}^*(s) = \Gamma(s)\mathbf{G}(s)$. Then

$$\mathbf{B}(s) = (\mathbf{I} - \mathbf{P}(s))^{-1}(\mathbf{B}(s-1) + \mathbf{G}(s)).$$

The quantity $(\mathbf{I} - \mathbf{P}(s))^{-1}$ has a pole at $s = -1$. Together with $\Gamma(s)$ it would give a double pole at $s = -1$ which is not possible, as proved above. Indeed, notice that the coefficient at the double pole at $s = 1$ is $\mathbf{\Pi}(\mathbf{B}(-2) + \mathbf{G}(-1)$. But $\mathbf{G}(-1)$ is the the coefficient at z of $\mathbf{g}(z)$ and $\mathbf{B}(-2)$ is the coefficient at z^2 of $\mathbf{V}(z)$, as already proved in Lemma 12. Then we easily see that $\mathbf{B}(-2) + \mathbf{G}(-1) = \mathbf{P}^2\mathbf{e}_a - \mathbf{P}\mathbf{e}_a$, and consequently the coefficient at the double pole at $s = 1-$ is equal to $\mathbf{\Pi}(\mathbf{P}^2\mathbf{e}_a - \mathbf{P}\mathbf{e}_a) = (\mathbf{\Pi} - \mathbf{\Pi})\mathbf{e}_a = 0$, as desired.

Therefore, the contribution of pole $s = -1$ to the asymptotic of $\mathbf{V}(z)$ is $\mathbf{B}(-1)$ becomes

$$\begin{aligned}\mathbf{B}(-1) \quad = \quad & \frac{1}{\lambda'(-1)}\left(\langle \boldsymbol{\pi}'(-1)(\mathbf{B}(-2) + \mathbf{G}(-1))\rangle + \langle \boldsymbol{\pi}(\mathbf{B}'(-2) + \mathbf{G}'(-1))\rangle\right)\mathbf{1} \\ & + (\mathbf{I} - \mathbf{R}(-1))^{-1}(\mathbf{B}(-2) + \mathbf{G}(-1)).\end{aligned}$$

Notice also that $(\mathbf{I}-\mathbf{R}(-1))^{-1}(\mathbf{P}^2\mathbf{e}_a-\mathbf{P}\mathbf{e}_a)=\langle\boldsymbol{\pi}\mathbf{P}\mathbf{e}_a\rangle\mathbf{1}-\mathbf{P}\mathbf{e}_a=\langle\boldsymbol{\pi}\mathbf{e}_a\rangle\mathbf{1}-\mathbf{P}\mathbf{e}_a$.

The real issue here is how to compute $\mathbf{B}'(-2)$ and $\mathbf{G}'(-1)$, which we address next.

▶ **Lemma 13.** *Let a function $g(z)=\sum_{n\geq 1}\frac{a_n}{n!}z^n$ and $f(z)=g(z)e^{-z}=\sum_{n\geq 1}\frac{b_n}{n!}z^n$. Let also $g_k(z)=\sum_{n\leq k}\frac{a_n}{n!}z^n$ and $f_k(z)=f(z)-g_k(z)e^{-z}$ with $f_k^*(s)$ being its Mellin transform defined for $-k-1<\Re(s)<0$. Then*

$$\begin{aligned}\lim_{s\to -k}\left(\frac{f^*(s)}{\Gamma(s)}\right)' &= f_k^*(-k)\left(\frac{1}{\Gamma(s)}\right)'_{s=-k}+\sum_{n\leq k}\frac{a_n}{n!}\left(s^{\langle n\rangle}\right)'_{s=-k}\\ &= f_k^*(-k)(-1)^{n-1}n!+\sum_{n\leq k}\frac{a_n}{n!}\left(s^{\langle n\rangle}\right)'_{s=-k}\end{aligned}$$

where $s^{\langle n\rangle}=\frac{\Gamma(s+n)}{\Gamma(s)}=(s+n-1)\times\cdots\times s$.

Proof. We start with a simple identity

$$\frac{f^*(s)-f_k^*(s)}{\Gamma(s)}=\sum_{n\leq k}\frac{a_n}{n!}s^{\langle n\rangle}$$

which is easy to derive. But the Mellin transform of $f_k(z)$ and $f_k^*(s)$ are defined for $-k-1<\Re(s)<0$. The derivative of $f_k^*(s)/\Gamma(s)$ at $s=-k$ is equal to $f_k^*(-k)\left(\Gamma^{-1}(s)\right)'_{s=-k}$ since $\Gamma^{-1}(-k)=0$. Finally we notice that [15]

$$\lim_{s\to -k}\left(\frac{1}{\Gamma(s)}\right)'=\lim_{s\to -k}\frac{\Psi(s)}{\Gamma(s)}=\lim_{s\to -k}\frac{(s+n)\Psi(s)}{(s+n)\Gamma(s)}=(-1)^{n-1}n!$$

where $\Psi(s)$ is the psi function. ◀

In absence of specific properties on $f_k(z)$ there is no other way than numerical computation to get an estimate of $f_k^*(-k)$. Finally, we can present a precise asymptotic expression for the variance.

▶ **Theorem 14.** *We have $\boldsymbol{V}(z)=\bar{\omega}_a\boldsymbol{1}z+o(z)$ in the aperiodic case, and in the periodic case $\boldsymbol{V}(z)=\bar{\omega}_a\boldsymbol{1}z+Q_2(\log z)z+O(z^{1-\epsilon})$ for some $\epsilon>0$ and $Q_2(.)$ being a periodic function of small amplitude and mean zero, where*

$$\bar{\omega}_a=\frac{1}{\lambda'(-1)}\left(\langle\boldsymbol{\pi}'(-1)((\boldsymbol{P}-\boldsymbol{I})\boldsymbol{P}\boldsymbol{e}_a\rangle+\langle\boldsymbol{\pi}(\boldsymbol{B}'(-2)+\boldsymbol{G}'(-1))\rangle\right)+\langle\boldsymbol{\pi}\boldsymbol{e}_a\rangle. \tag{B.16}$$

Notice that $\omega=B(-1)+\boldsymbol{P}\boldsymbol{e}_a$.

Power-Law Degree Distribution in the Connected Component of a Duplication Graph

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Abstract

We study the partial duplication dynamic graph model, introduced by Bhan et al. in [3] in which a newly arrived node selects randomly an existing node and connects with probability p to its neighbors. Such a dynamic network is widely considered to be a good model for various biological networks such as protein-protein interaction networks. This model is discussed in numerous publications with only a few recent rigorous results, especially for the degree distribution. Recently Jordan [9] proved that for $0 < p < \frac{1}{e}$ the degree distribution of the *connected component* is stationary with *approximately* a power law. In this paper we rigorously prove that the tail is indeed a true power law, that is, we show that the degree of a randomly selected node in the connected component decays like C/k^{β} where C an explicit constant and $\beta \neq 2$ is a non-trivial solution of $p^{\beta-2} + \beta - 3 = 0$. This holds regardless of the structure of the initial graph, as long as it is connected and has at least two vertices. To establish this finding we apply analytic combinatorics tools, in particular Mellin transform and singularity analysis.

2012 ACM Subject Classification Mathematics of computing → Random graphs; Theory of computation → Random network models

Keywords and phrases random graphs, pure duplication model, degree distribution, tail exponent, analytic combinatorics

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.16

Funding This work was supported by NSF Center for Science of Information (CSoI) Grant CCF-0939370, in addition by NSF Grant CCF-1524312, and National Science Center, Poland, Grant 2018/31/B/ST6/01294.

1 Introduction

Recent years have seen a growing interest in dynamic graph models [10]. These models are often claimed to describe well various real-world structures, such as social networks, citation networks and various biological data. For example, protein-protein are widely viewed as driven by an internal evolution mechanism based on duplication and mutation. In this case, new nodes are added to the network as copies of existing nodes together with some random divergence. It has been claimed that graphs generated from these models exhibit many properties characteristic for real-world networks such as power-law degree distribution, the large clustering coefficient, and a large amount of symmetry [4]. However, some of these results turned out not to be correct; in particular, the power-law degree distribution was

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 16; pp. 16:1–16:14
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

disproved in [7]. In this paper we focus on the tail distribution of the *connected component* of such networks and show rigorously the existence of a power law improving and making more precise recent result of Jordan [9].

The model analyzed in this paper is known as the *partial (pure) duplication model*, in which a new node selects an existing node and connects to its neighbors with probability p. More precisely, the model is defined formally as follows: let $0 < p \leq 1$ be the only parameter of the model. In discrete steps repeat the following procedure: first, choose a single vertex u uniformly at random. Then, add a new vertex v and for all vertices w such that uw is an edge (i.e., w is a neighbor of u) flip a coin independently at random (heads with probability p, tails with $1 - p$) and add vw edge if and only if we got heads. The partial duplication model was defined by Bhan et al. in [3] and then was further studied in [1, 4, 7, 9, 8].

The case when $p = 1$, also called the *full duplication model*, was analyzed recently in the context of graph compression in [13]. In particular, it was formally proved that the expected logarithm of the number of automorphisms (symmetries) for such graphs on n vertices is asymptotically $\Theta(n \log n)$, which in turn lead us to an asymptotically efficient compression algorithm for such case.

The *partial duplication* case $0 < p < 1$ was given much more attention, however, with very few rigorous results. It was first and foremost analyzed to find the stationary distribution of the degree, that is,

$$f_k = \lim_{n\to\infty} f_k(n) = \lim_{n\to\infty} \frac{F_k(n)}{n} = \lim_{n\to\infty} \Pr[\deg(U_n) = k],$$

where $f_k(n)$ and $F_k(n)$ are, respectively, the average fraction and the average number of vertices of degree k in a graph generated by this model and U_n is a random variable denoting a vertex chosen uniformly at random from a graph on n vertices generated from the partial duplication model. Hermann and Pfaffelhuber in [7] proved that this process $(f_k(n))_{n=n_0}^{\infty}$ converges always to the limit $f_0 = 1$ and $f_k = 0$ for all other k when $p \leq p^* = 0.57\ldots$ (that is, p^* being the unique root of $pe^p = 1$), regardless of the initial graph. They have also shown that if $p > p^*$ there exists only a defective distribution of the degrees with $f_0 = c < 1$ for a certain constant c (depending on the initial graph) and $f_k = 0$ for all other k. For the average degree distribution see also [14].

This result, although it refuted the power law behavior of the whole graph claimed by [4, 2], also showed that asymptotically almost all vertices are isolated. This has still left the possibility that it might be the case that a graph generated by the partial duplication model with the isolated vertices removed exhibits such property. Note that by a simple inductive argument it is obvious that if a vertex is isolated at the time of its insertion, then it stays isolated forever, and if it was connected to other vertex, then it remains connected, so if the inital graph is connected, then there can only be one component containing all non-isolated vertices. This was exactly the route pursued by Jordan in [9]. Using probabilistic tools such as the quasi-stationary distribution of a certain continuous time Markov chain embedding of the original discrete graph growth process, Jordan was able to prove that for $0 < p < \frac{1}{e}$ there is an *approximate power law* behavior in the pure duplication graphs. More precisely, let us define for a vertex (denoted by U_n) picked uniformly at random from a graph on n vertices generated from the duplication model the following conditional probability

$$a_k(n) = \Pr[\deg(U_n) = k | \deg(U_n) \neq 0] = \frac{f_k(n)}{\sum_{i=1}^{\infty} f_i(n)} = \frac{f_k(n)}{1 - f_0(n)}. \tag{1}$$

Jordan proved that $a_k(n) \to a_k$ as $n \to \infty$ as long as the underlying process is positive recurrent which holds for $p < \frac{1}{e}$ [9]. Moreover, Jordan showed that for $\beta(p) \neq 2$ being the solution of $p^{\beta-2} + \beta - 3 = 0$ the tail behavior of a_k is approximately a power law in the sense that it is lighter than any heavier tailed power law (with any index $\beta(p)+\varepsilon$, $\varepsilon > 0$) and heavier than any lighter tailed power law (with index $\beta(p)-\varepsilon$, $\varepsilon > 0$). This is of vital interest in this area since $\beta(p) \in (2,3)$, which is exactly the range of the power law exponents for various real-world biological graphs, such as protein-protein newtorks [4].

It is worth noting that it partially confirmed the non-rigorous result by Ispolatov et al. from [8], who claimed that the connected component exhibits a power-law distribution both for $0 < p < \frac{1}{e}$ (with index $\beta(p)$ as above), and for $\frac{1}{e} \le p < \frac{1}{2}$ (with index 2). Furthermore, by the virtue of (1) observe, following [9, 7], that $f_0(n) = 1 - o(1)$ and $f_k(n) = o(1)$ for $k \ge 1$ which begs the question of the asymptotic behavior of $f_k(n)$ for large k and n. Certainly $f_k(n)$ does *not* grow linearly with n as suggested in some papers (cf. [2]). We conjecture that $f_k(n) = O(n^{-\alpha(p)}k^{-\beta(p)})$ for some $1 < \alpha(p) < 2$ and $\beta(p) > 2$, but this problem is left for future research.

In this paper we finally establish the precise behavior of the tail of the degree distribution for pure duplication model for $0 < p < \frac{1}{e}$ completing the work of Jordan [9]. More precisely, we use tools of analytic combinatorics such as the Mellin transform and singularity analysis to prove in Theorem 2 that the tail of a node degree in the connect component of the partial duplication model decays as $C/k^{\beta(p)}$ where C an explicit constant.

The paper is organized as follows: in Section 2 we present a formal definition of the model, introduce the tracked vertex approach, and the quasi-stationary distribution as defined by Jordan in [9]. In Section 3 we state and establish our main results using Mellin transform and singularity analysis. In concluding Section 4 we indicate a possible extension of our findings and point to some further work.

2 The model and Jordan's approach

We follow the standard graph-theoretical notation, e.g., from [5]. We consider only simple graphs, i.e., graphs without loops or parallel edges.

Let us recall first the definition of the pure duplication model. Let $G_{n_0} = (V_{n_0}, E_{n_0})$ be an initial graph with a set of vertices V_{n_0} and a set of edges E_{n_0}, such that $|V_{n_0}| = n_0 \ge 2$. Throughout the paper, let us assume that G_{n_0} is fixed and connected. For $n = n_0, n_0+1, \ldots$ we build $G_{n+1} = (V_{n+1}, E_{n+1})$ from $G_n = (V_n, E_n)$ in the following way:

1. pick a vertex $u \in V_n$ uniformly at random,
2. create a new node v_{n+1} and let $V_{n+1} = V_n \cup \{v_{n+1}\}$, $E_{n+1} = E_n$,
3. for every $w \in V_n$ such that $uw \in E_n$ add edge $v_{n+1}w$ to E_{n+1} independently at random with probability p.

We call the process $\mathcal{G} = (G_n)_{n=n_0}^{\infty}$ the *partial duplication graph*.

Jordan in [9] introduced the continuous-time embedding of this process, defined as following: start at time $t = 0$ with a fixed connected graph $\Gamma_0 = G_{n_0}$ and let $(\Gamma_t)_{t\ge 0}$ be a continuous time Markov chain on graphs, where each vertex is duplicated independently at times following a Poisson process of rate 1, with the rules for duplication as in the pure duplication model.

Jordan also defined the so called *vertex tracking approach*: we pick a vertex from Γ_0 uniformly at random and then define the continuous-time process $(V_t)_{t\ge 0}$ in the following way: at time t we jump to a vertex v if and only if the vertex V_{t-} was duplicated and its „child" is v. He proved that for any $k \ge 1$ and for another continuous-time process $(U_t)_{t\ge 0}$ being defined as a uniform choice of vertices over Γ_t we have

$$\lim_{t\to\infty} \frac{\Pr[\deg(U_t) = k]}{\Pr[\deg(V_t) = k]} = 1.$$

Therefore, asymptotically the behavior of a tracked vertex approximates the behavior of a random vertex in Γ_t when $t \to \infty$, and therefore in G_n when $n \to \infty$.

The tracked vertex approach allowed Jordan to construct the generator Q of the continuous-time Markov chain $(\deg(V_t))_{t\geq 0}$, defined over the state space $\mathbb{N}_0$, with the following transitions

$$\begin{aligned} q_{j,k} &= \binom{j}{k} p^k (1-p)^{j-k} && \text{for } 0 \leq k \leq j-1, \\ q_{j,j} &= -jp - \left(1-p^j\right), \\ q_{j,j+1} &= jp. \end{aligned}$$

Then Jordan proceeded to the analysis of the quasi-stationary distribution $(a_k)_{k=1}^{\infty}$, i.e., the left eigenvector of a subset of Q, defined as before. We relate this distribution to the eigenvalue $-\lambda$ (see [11] for details of this approach) being the solution of the equation $AQ = -\lambda Q$, where $A = (a_k)_{k=1}^{\infty}$. This leads us to the following equation:

$$\sum_{j=k}^{\infty} a_j \binom{j}{k} p^k (1-p)^{j-k} = -(k-1)pa_{k-1} - (\lambda - kp - 1)\, a_k \tag{2}$$

for $k = 1, 2, 3, \ldots$.

Using (2) and the generating function $A(z) = \sum_{k=0}^{\infty} a_k z^k$ Jordan found the following differential-functional equation

$$A(pz + 1 - p) = (1-\lambda)A(z) + pz(1-z)A'(z) + A(1-p). \tag{3}$$

Notice that the above equation implies that $A(0) = 0$. Since it is a sum of limits for probability distributions, by Fatou's lemma $|A(z)| \leq 1$ for $|z| \leq 1$. By letting $z \to 1^-$ in (3) and assuming finite $A'(1)$ we get $A(1-p) = \lambda A(1)$.

Furthermore with the identity

$$A'(z) = \frac{A(pz+1-p) - A(1)}{pz(1-z)} - (1-\lambda)\frac{A(z) - A(1)}{pz(1-z)} \tag{4}$$

and letting $z \to 1^-$ Jordan found

$$A'(1) = -A'(1) + \frac{1-\lambda}{p} A'(1),$$

namely, if $A'(1)$ is non-zero and finite, then $\lambda = 1 - 2p$. Finally, using the assumptions that the distribution $(a_k)_{k=0}^{\infty}$ is non-degenerate (i.e., $\sum_{k=0}^{\infty} a_k = A(1) = 1$) and that the mean degree $A'(1)$ is finite, Jordan found that for $0 < p < \frac{1}{e}$ the quasi-stationary distribution a_k does not have q-th moment for $p^{q-2} + q - 3 < 0$.

In summary Jordan proved the following result.

▶ **Theorem 1** ([9, Theorem 2.1(3)]). *Assume $0 < p < \frac{1}{e}$. Let $\beta(p) > 2$ be the solution of $p^{\beta-2} + \beta - 3 = 0$. Then the tail behaviour of $(a_k)_{k=0}^{\infty}$ has a power law of index $\beta(p)$, in the sense that as $k \to \infty$,*

$$\begin{aligned} \lim_{k\to\infty} \frac{a_k}{k^q} &= 0 \quad \textit{for } q < \beta(p), \\ \lim_{k\to\infty} \frac{a_k}{k^q} &= \infty \quad \textit{for } q > \beta(p). \end{aligned}$$

In the next section we present our refinement of this theorem and provide precise asymptotics for $(a_k)_{k=0}^{\infty}$.

3 Main results

In this section we state and prove the main result of our paper that is a refinement of Theorem 1.

▶ **Theorem 2.** *If $0 < p < \frac{1}{e}$, then the stationary distribution $(a_k)_{k=0}^{\infty}$ of the pure duplication model has the following asymptotic tail behavior as $k \to \infty$:*

$$\frac{a_k}{k^{\beta(p)}} = \frac{1}{E(1) - E(\infty)} \cdot \frac{p^{-\frac{1}{2}(\beta(p)-\frac{3}{2})^2}\Gamma(\beta(p)-2)}{D(\beta(p)-2)(p^{-\beta(p)+2}+\ln(p))\Gamma(-\beta(p)+1)} \left(1 + O\left(\frac{1}{k}\right)\right) \quad (5)$$

where $\beta(p) > 2$ is the non-trivial solution of $p^{\beta-2} + \beta - 3 = 0$, $\Gamma(s)$ is the Euler gamma function and

$$D(s) = \prod_{i=0}^{\infty} \left(1 + p^{1+i-s}(s-i-2)\right), \quad (6)$$

$$E(1) - E(\infty) = \frac{1}{2\pi i} \int_{\mathrm{Re}(s)=c} p^{-\frac{1}{2}(s-\frac{1}{2})^2} \frac{\Gamma(s)}{D(s)} \,\mathrm{d}s, \quad \textit{for } c \in (0,1).$$

In Figure 1 we present numerical values of the functions involved in the formula above. It clear that that all coefficients in (5) are positive for $0 < p < \frac{1}{e}$.

The rest of this section is devoted to the proof of our main result. We will accomplish it by a series of lemmas. The main idea is as follows: we take (3) and apply a series of substitutions to obtain a functional equation which is in suitable form for applying Mellin transform. Observe that we cannot apply directly Mellin transform to the functional equation (5) due to the term $A(pz + 1 - p)$.

It is already known from [9] that $A'(1)$ is non-zero and finite, hence $\lambda = 1 - 2p$. First, let us substitute $z = 1 - v$ and $B(v) = A(1 - v)$ in (3). Thus

$$A(1 - pv) = 2pA(1 - v) + pv(1 - v)A'(1 - v) + A(1 - p),$$
$$B(pv) = 2pB(v) - pv(1 - v)B'(v) + A(1 - p).$$

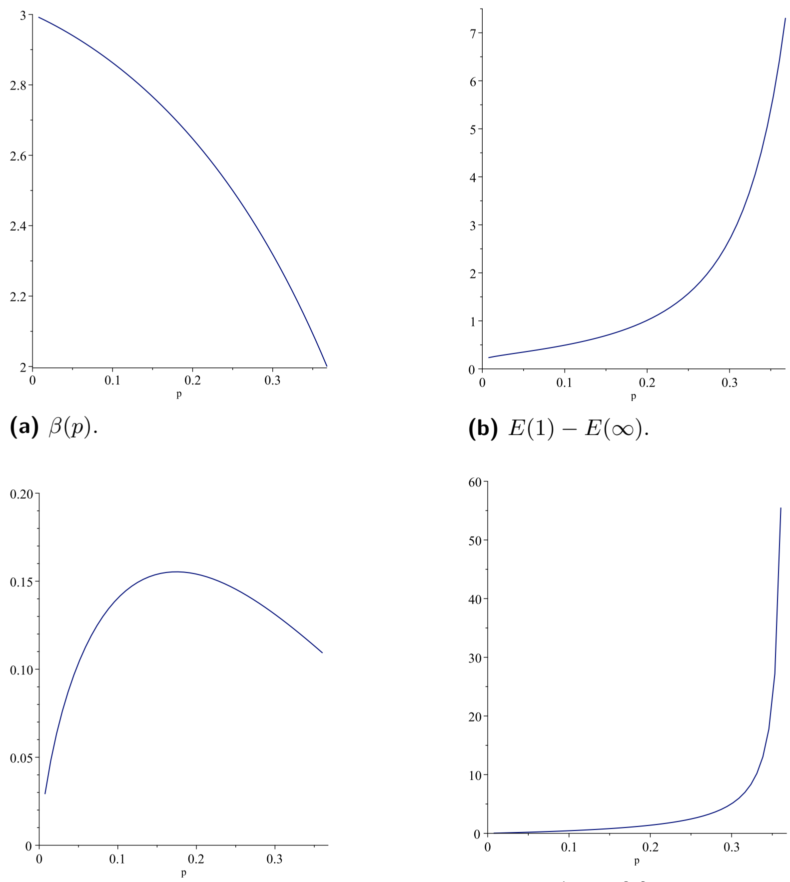
Observe now that the functional equation on $B(v)$ is suitable for the Mellin transform. To ease some computation let $w = \frac{1}{v}$ and $C(w) = B\left(\frac{1}{w}\right)$. Then

$$B\left(\frac{p}{w}\right) = 2pB\left(\frac{1}{w}\right) - \frac{p}{w}\left(1 - \frac{1}{w}\right)B'\left(\frac{1}{w}\right) + A(1 - p),$$
$$C\left(\frac{w}{p}\right) = 2pC(w) + p(w - 1)C'(w) + A(1 - p). \quad (7)$$

Therefore, we are essentially looking at the solution of (7) with boundary conditions $C(1) = A(0) = 0$ and $\lim_{w\to\infty} C(w) = A(1)$ (which is equal to 1, as pointed out in [9]).

Our objective is to find an asymptotic expansion for $C(w)$ when $w \to \infty$. Notice that it is equivalent to finding the asymptotic expansion of $A(z)$ when $z \to 1$ by inferior values. For this purpose we will use the Mellin transform which is a powerful tool for extracting accurate asymptotic expansions [12]. Unfortunately we cannot directly apply the Mellin transform over function $C(w)$ since the behavior of $C(w)$ for $w \to 0$ is yet unknown. To circumvent this problem we search for a similar function $E(w)$ defined by the following functional equation

$$E\left(\frac{w}{p}\right) = 2pE(w) + p(w - 1)E'(w) + K \quad (8)$$



(a) $\beta(p)$. **(b)** $E(1) - E(\infty)$.

(c) $D(\beta(p) - 2)$. **(d)** $\frac{p^{-\frac{1}{2}(\beta(p)-\frac{3}{2})^2}\Gamma(\beta(p)-2)}{\left(p^{-\beta(p)+2}+\ln(p)\right)\Gamma(-\beta(p)+1)}$.

Figure 1 Numerical values of different parts of (3) for $0 < p < \frac{1}{e}$.

for some constant K for which we shall postulate that the Mellin transform

$$E^*(s) = \int_0^\infty w^{s-1} E(w)\,\mathrm{d}w$$

exists in some fundamental strip.

To connect $E(w)$ with our function $C(w)$ we notice that it holds necessarily that $C(1) = 0$ which corresponds to the fact that $A(0) = 0$. Clearly, if $E(w)$ is the solution of (8) with finite values of both $E(1)$ and $E(\infty) = \lim_{w\to\infty} E(w)$ (which will be shown later to be the case), then it is also true that

$$C(w) = A(1)\frac{E(w) - E(1)}{E(\infty) - E(1)} \tag{9}$$

is the solution of (7) with $C(1) = 0$ which also satisfies $\lim_{w\to\infty} C(w) = A(1) = 1$.

Let us now proceed through definition and lemmas. We first define

$$E^*(s) = p^{-\frac{1}{2}(s-\frac{1}{2})^2}\frac{\Gamma(s)}{D(s)} \tag{10}$$

for $D(s) = \prod_{j=0}^{\infty}\left(1 + p^{1+j-s}(s - j - 2)\right)$ defined already in (6).

Now notice that $D(s) = 0$ implies $1 + p^{1+j-s}(s - j - 2) = 0$ for some $j \in \mathbb{N}$. This equation for $0 < p < \frac{1}{e}$ has only two solutions: $s = j + 1$ and $s = j + 1 + s^*$, where s^* is the non-trivial (i.e. other than $s = 0$) solution of $p^s + s - 1 = 0$.

Therefore, $E^*(s)$ has only simple, isolated poles of three types:

- for $s = 0, -1, -2, \ldots$, introduced by $\Gamma(s)$,
- for $s = 1, 2, 3, \ldots$, introduced by $\frac{1}{D(s)}$,
- for $s = s^* + 1, s^* + 2, s^* + 3, \ldots$, introduced by $\frac{1}{D(s)}$.

Moreover, if we omit these poles, then $D(s)$ converges to a non-zero finite value when $\mathrm{Re}(s) < 0$ because p^{i-s} exponentially decays. We summarize it in the next lemma.

▶ **Lemma 3.** *For* $\mathrm{Re}(s) \in (-1, 0)$ *and* $0 < p < \frac{1}{e}$ *it holds that* $\frac{1}{|D(s)|}$ *is absolutely convergent.*

Due to its technical intricacies, the proof of Lemma 3 was moved to the Appendix. In Figure 2 we present an example plot of values of $\frac{1}{|D(s)|}$.

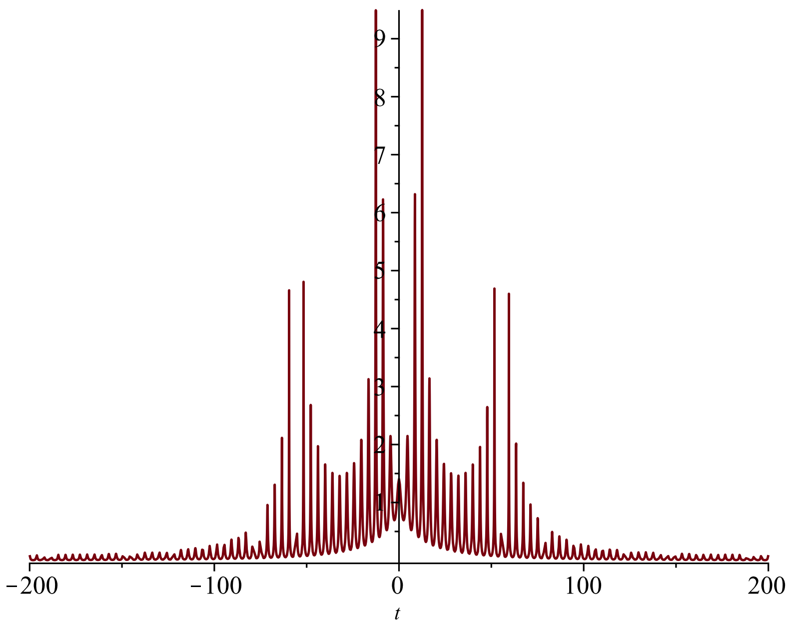


Figure 2 Numerical values of $\frac{1}{|D(c+it)|}$ for $p = 0.2$ and $c = -0.5$.

▶ **Lemma 4.** *For* $0 < p < \frac{1}{e}$ *it holds that*

$$E^*(s) = \frac{p(s-1)}{p^s + ps - 2p} E^*(s-1).$$

Proof. We have the identity

$$\frac{p^{\frac{1}{2}(s-\frac{1}{2})^2}}{\Gamma(s)} E^*(s) = \frac{p^{\frac{1}{2}(s-\frac{3}{2})^2}}{\Gamma(s-1)} E^*(s-1) \frac{1}{1 + p^{1-s}(s-2)}.$$

Thus

$$E^*(s) = \frac{p^{-\frac{1}{2}(s-\frac{1}{2})^2 + \frac{1}{2}(s-\frac{3}{2})^2}}{1 + p^{1-s}(s-2)} \frac{\Gamma(s)}{\Gamma(s-1)} E^*(s-1) = \frac{p^{1-s}}{1 + p^{1-s}(s-2)} (s-1) E^*(s-1)$$

since $\frac{\Gamma(s)}{\Gamma(s-1)} = s - 1$. Multiplying by numerator and denominator by p^s completes the proof. ◀

We now define for any given $c \in (-1, 0)$

$$E(w) = \frac{1}{2\pi i}\int_{\mathrm{Re}(s)=c} E^*(s) w^{-s}\,\mathrm{d}s = \frac{1}{2\pi i}\int_{\mathrm{Re}(s)=c} p^{-\frac{1}{2}(s-\frac{1}{2})^2}\frac{\Gamma(s)}{D(s)} w^{-s}\,\mathrm{d}s. \tag{11}$$

Notice that this integral converges for any complex value of w with $\mathrm{Im}(w) \to \pm\infty$ because from Lemma 3 it follows that $\frac{1}{|D(s)|}$ is bounded by a constant and $\Gamma(s)p^{-\frac{1}{2}(s-\frac{1}{2})^2}$ decays faster than any polynomial. Furthermore the value of $E(w)$ does not depend on the value of quantity c thanks to Cauchy's theorem.

▶ **Lemma 5.** *The function $E(w)$ has function $E^*(s)$ as its Mellin transform with its fundamental strip being $\{s : \mathrm{Re}(s) \in (-1, 0)\}$.*

Proof. We have

$$|E(w)| \leq \frac{|w|^{-c}}{2\pi}\int_{-\infty}^{+\infty} |E^*(c+it)| \exp(\arg(w)t)\,\mathrm{d}t.$$

Now, it is easy to spot that $E(c+it) = O\left(\exp\left(-\frac{t^2}{2}\right)\right)$ since $\ln(p) < -1$, thus the integral $\int_{-\infty}^{+\infty} |E^*(c+it)| \exp(\arg(w)t)\,\mathrm{d}t$ absolutely converges and it follows that $E(w) = O(w^{-c})$. Since it is true for any values of $c \in (-1, 0)$ when $w \to 0$ and $w \to \infty$, then the Mellin transforms of function $E(w)$ exists with the fundamental strip $\{s : \mathrm{Re}(s) \in (-1, 0)\}$.

Furthermore, its Mellin transform is $E^*(s)$ because (11) is exactly the inverse Mellin transform formula. ◀

▶ **Lemma 6.** *There exists a value K independent of w such that*

$$R(w) = -\operatorname{Res}\big[E^*(s-1)p(s-1)w^{-s}, s = 0\big] = -K.$$

Proof. The expression

$$R(w) = E\left(\frac{w}{p}\right) - 2pE(w) - p(w-1)E'(w)$$

can be also expressed via an integral as

$$R(w) = \frac{1}{2\pi i}\int_{\mathrm{Re}(s)=c} E^*(s)\left(p^s w^{-s} - 2pw^{-s} + spw^{-s} - spw^{-s-1}\right)\mathrm{d}s$$

which can be rewritten as follows

$$\begin{aligned}
R(w) &= \frac{1}{2\pi i}\int_{\mathrm{Re}(s)=c} E^*(s)\left(p^s - 2p + ps\right) w^{-s}\,\mathrm{d}s \\
&\quad - \frac{1}{2\pi i}\int_{\mathrm{Re}(s)=c+1} E^*(s-1)p(s-1)w^{-s}\,\mathrm{d}s \\
&= \frac{1}{2\pi i}\int_{\mathrm{Re}(s)=c} \left(\left(p^s + ps - 2p\right)E^*(s) - p(s-1)E^*(s-1)\right) w^{-s}\,\mathrm{d}s \\
&\quad - \operatorname{Res}[p(s-1)E^*(s-1), s = 0]
\end{aligned}$$

since

$$\int_{\mathrm{Re}(s)=c+1} p(s-1)E^*(s-1)w^{-s}\,\mathrm{d}s - \int_{\mathrm{Re}(s)=c} p(s-1)E^*(s-1)w^{-s}\,\mathrm{d}s$$

define a contour path which encircles a simple pole at $s = 0$ in the counter-clockwise (i.e., positive) direction.

Furthermore from Lemma 3 it follows that

$$(p^s + ps - 2p)E^*(s) - p(s-1)E^*(s-1) = 0,$$

therefore the integral vanishes and finally $R(w) = -\operatorname{Res}[p(s-1)E^*(s-1), s=0] = -K$ for some constant K independent of w. ◀

▶ **Lemma 7.** *It holds that*

$$K = -\frac{p^{-\frac{1}{8}}(1-2p)}{D(0)}, \qquad E(\infty) = \frac{p^{-\frac{1}{8}}}{D(0)}.$$

Furthermore,

$$E(\infty) - E(1) = -\frac{1}{2\pi i}\int_{\operatorname{Re}(s)=c} E^*(s)\,\mathrm{d}s, \quad \text{for } c \in (0,1). \tag{12}$$

Proof. From Lemma 6 we have

$$K = \operatorname{Res}[p(s-1)E^*(s-1), s=0] = \frac{p^{-\frac{1}{8}}}{D(-1)}.$$

Moreover, from the definition $D(0) = (1-2p)D(-1)$, which establishes the first identity.

To find an expression for $E(\infty)$ is a little more delicate. Indeed from (11) we find

$$E(w) = -\operatorname{Res}\big[E^*(s)w^{-s}, s=0\big] + \frac{1}{2\pi i}\int_{\operatorname{Re}(s)=c'} E^*(s)w^{-s}\,\mathrm{d}s$$

by assuming the contour path is moved right to origin for some $c' \in (0,1)$. It turns out that 0 is the simple pole encountered in the move, as $D(s) \neq 0$ for all other s with $\operatorname{Re}(s) \in (0,1)$.

Furthermore, the integral on $\operatorname{Re}(s) = c'$ is in $O(w^{-c'})$ as $w \to \infty$, which allows to conclude that $E(w) = -\operatorname{Res}[E^*(s)w^{-s}, s=0] + O(w^{-c'})$ with $c' \in (0,1)$, thus

$$E(\infty) = \lim_{w\to\infty} E(w) = -\lim_{w\to\infty}\operatorname{Res}\big[E^*(s)w^{-s}, s=0\big] = -\operatorname{Res}[E^*(s), s=0] = -\frac{p^{-\frac{1}{8}}}{D(0)}.$$

Finally,

$$E(\infty) - E(1) = -\operatorname{Res}[E(s), s=0] - \frac{1}{2\pi i}\int_{\operatorname{Re}(s)=c} E^*(s)\,\mathrm{d}s = -\frac{1}{2\pi i}\int_{\operatorname{Re}(s)=c'} E^*(s)\,\mathrm{d}s$$

for, respectively, $c \in (-1,0)$ and $c' \in (0,1)$ since

$$\frac{1}{2\pi i}\int_{\operatorname{Re}(s)=c'} E^*(s)\,\mathrm{d}s - \frac{1}{2\pi i}\int_{\operatorname{Re}(s)=c} E^*(s)\,\mathrm{d}s = \operatorname{Res}[E(s), s=0].$$

This completes the proof. ◀

Note that $D(0) > 0$ since every element in the product is positive for $0 < p < \frac{1}{e}$. Therefore $K > 0$ and $E(\infty) < 0$.

Finally we proceed with the proof of the main theorem.

Proof of Theorem 2. Recall the observation that $E^*(s)$ has poles for $s \in \{1,2,\ldots\} \cup \{s^*+1, s^*+2,\ldots\} \cup \{0,-1,-2,\ldots\}$, for s^* – the non-zero solution of $p^s + s - 1 = 0$. Note that if $0 < p < \frac{1}{e}$, then $s^* > 0$.

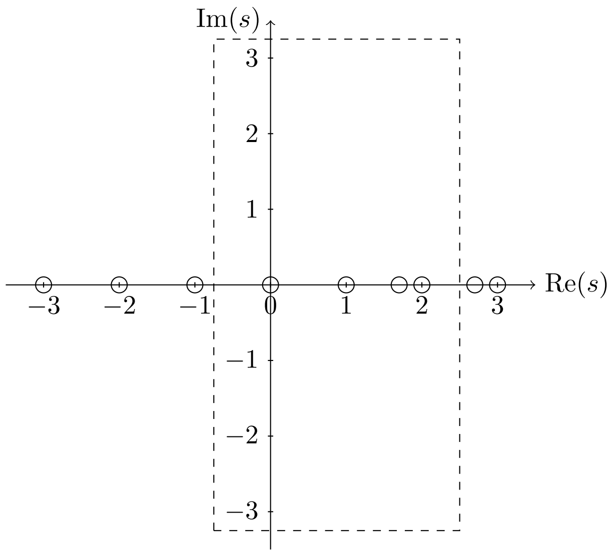


Figure 3 Example integration area for $E^*(s)$ and $E(w)$ with $s^* = 0.7$ and $M = 2.5$.

Therefore, for any $c \in (-1, 0)$ and a rectangle as presented in Figure 3, we are in position to write

$$\begin{aligned} C(w) &= \frac{1}{E(\infty) - E(1)} \frac{1}{2\pi i} \int_{\mathrm{Re}(s)=c} E^*(s) w^{-s} \, \mathrm{d}s - \frac{E(1)}{E(\infty) - E(1)} \\ &= -\frac{1}{E(\infty) - E(1)} \left(E(1) + \mathrm{Res}[E^*(s), s = 0] + \mathrm{Res}\big[E^*(s) w^{-s}, s = 1\big]\right) \\ &\quad - \frac{1}{E(\infty) - E(1)} \left(\mathrm{Res}\big[E^*(s) w^{-s}, s = 2\big] + \mathrm{Res}\big[E^*(s) w^{-s}, s = s^* + 1\big]\right) \\ &\quad + \frac{1}{E(\infty) - E(1)} \frac{1}{2\pi i} \int_{\mathrm{Re}(s)=M} E^*(s) w^{-s} \, \mathrm{d}s \end{aligned} \tag{13}$$

for any number $M \in (2, 2 + s^*)$.

The quantity

$$\frac{1}{2\pi i} \int_{\mathrm{Re}(s)=M} E^*(s) w^{-s} \, \mathrm{d}s = O(w^{-M})$$

since $w^{-s} = w^{-M} w^{-\mathrm{Im}(s)}$ and the integral in $E^*(s) w^{-\mathrm{Im}(s)}$ absolutely converge. Again this holds by a similar argument that was used in Lemma 3: $p^{-\frac{1}{2}(s-\frac{1}{2})^2}$ decays exponentially faster than $\frac{\Gamma(s)}{D(s)} w^{\mathrm{Im}(s)}$ for complex s.

By virtue of the residue theorem

$$\begin{aligned} C(w) &= -\frac{1}{E(\infty) - E(1)} \left(E(1) + \mathrm{Res}[E^*(s), s = 0] + \mathrm{Res}[E^*(s), s = 1] w^{-1}\right) \\ &\quad - \frac{1}{E(\infty) - E(1)} \left(\mathrm{Res}[E^*(s), s = 2] w^{-2} + \mathrm{Res}[E^*(s), s = s^* + 1] w^{-1-s^*}\right) \\ &\quad + O(w^{-M}). \end{aligned} \tag{14}$$

This formula gives us an asymptotic expansion of $C(w)$ up to order w^{-M} where $M \in (2, 2+s^*)$.

In fact, for more precise computations it is possible an expansion to any desired value M, just by including all the residues of the poles in k ($k \in \mathbb{N}$) and $k + s^*$ ($k \in \mathbb{N}_+$) which are smaller than M as for $0 < p < \frac{1}{e}$ all poles are simple.

Next, there are computed the first residues, e.g.,

$$\begin{aligned}
\operatorname{Res}\big[E^*(s)w^{-s}, s=0\big] &= \left[p^{-\frac{1}{2}(s-\frac{1}{2})^2}\frac{w^{-s}}{D(s)}\right]_{s=0} = \frac{p^{-\frac{1}{8}}}{D(0)} = -E(\infty),\\
\operatorname{Res}\big[E^*(s)w^{-s}, s=1\big] &= \left[\frac{p^{-\frac{1}{2}(s-\frac{1}{2})^2}\Gamma(s)}{p^{1-s}-(s-2)p^{1-s}\ln(p)}\frac{w^{-s}}{D(s-1)}\right]_{s=1}\\
&= \frac{p^{-\frac{1}{8}}}{1+\ln(p)}\frac{w^{-1}}{D(0)},\\
\operatorname{Res}\big[E^*(s)w^{-s}, s=s^*+1\big] &= \left[\frac{p^{-\frac{1}{2}(s-\frac{1}{2})^2}\Gamma(s)}{p^{1-s}-(s-2)p^{1-s}\ln(p)}\frac{w^{-s}}{D(s-1)}\right]_{s=s^*+1}\\
&= \frac{p^{-\frac{1}{2}(s^*+\frac{1}{2})^2}\Gamma(s^*)}{p^{-s^*}-(s^*-1)p^{-s^*}\ln(p)}\frac{w^{-s^*-1}}{D(s^*)}\\
&= \frac{p^{-\frac{1}{2}(s^*+\frac{1}{2})^2}\Gamma(s^*)}{p^{-s^*}+\ln(p)}\frac{w^{-s^*-1}}{D(s^*)}.
\end{aligned}$$

Observe that in the formulas above both 1 and s^*+1 are not the zeros of $p^{1-s}-(s-2)p^{1-s}\ln(p)$, so all the presented expressions have finite value.

Now it is the moment to use the classic Flajolet-Odlyzko transfer theorem [6] to (9) and (14) and obtain

$$\begin{aligned}
A(z) = 1 &- \frac{1}{E(\infty)-E(1)}\frac{p^{-\frac{1}{8}}}{1+\ln(p)}\frac{1-z}{D(0)}\\
&- \frac{1}{E(\infty)-E(1)}\frac{p^{-\frac{1}{2}(s^*+\frac{1}{2})}\Gamma(s^*)}{p^{-s^*}+\ln(p)}\frac{(1-z)^{1+s^*}}{D(s^*)}\\
&- \frac{1}{E(\infty)-E(1)}\operatorname{Res}[E^*(s), s=2](1-z)^2\\
&- \frac{1}{E(\infty)-E(1)}\operatorname{Res}[E^*(s), s=s^*+2](1-z)^{s^*+2} + o((1-z)^{2+s^*}).
\end{aligned}$$

Finally, $(1-z)^\alpha$ for $\alpha \in \mathbb{N}$ is a polynomial and does not contribute to the asymptotics. And for $\alpha \in \mathbb{R}_+ \setminus \mathbb{N}$ [6] it holds that

$$\begin{aligned}
&[z^k](1-z)^\alpha = \frac{k^{-\alpha-1}}{\Gamma(-\alpha)}\left(1+O\left(\frac{1}{k}\right)\right),\\
&[z^k]o(1-z)^\alpha = o(k^{-\alpha-1}).
\end{aligned}$$

This leads to the final result, which holds for large k:

$$\begin{aligned}
a_k &= [z^k]A(z)\\
&= -\frac{1}{E(\infty)-E(1)}\frac{p^{-\frac{1}{2}(s^*+\frac{1}{2})^2}\Gamma(s^*)}{(p^{-s^*}+\ln(p))\Gamma(-s^*-1)}\frac{1}{D(s^*)}k^{-s^*-2}\left(1+O\left(\frac{1}{k}\right)\right).
\end{aligned}$$

Note that since s^* is the non-trivial real solution of $p^s+s-1=0$, equivalently the exponent may be written as $\beta(p) = s^*+2$ – the the non-trivial (i.e., other than 2) real solution of the equation $p^{\beta-2}+\beta-3=0$.

Putting all the results together we obtain (5) of Theorem 2. Now it is sufficient to confirm that if $0 < p < \frac{1}{e}$, then the tail exponent $\beta(p) > 2$, which means that $A'(1)$ is indeed finite. This proves Theorem 2. ◀

4 Discussion

We proved rigorously the power-law behavior for asymptotic degree distribution of the connected component of the duplication graph $0 < p < \frac{1}{e}$. There remains therefore an open question whether the similar results may be obtained for $p \geq \frac{1}{e}$.

On the one hand, recall the non-rigorous claim in [8] that for $\frac{1}{e} \leq p < \frac{1}{2}$ the index of the power law is equal to 2. Interestingly, $\beta = 2$ is the largest solution of $p^{\beta-2} + \beta - 3 = 0$ for $p \geq \frac{1}{e}$.

On the other hand, Jordan [9, Proposition 3.7] has shown that the dual Markov chain with respect to the eigenvalue $\lambda = 1 - 2p$ is transient for all $p > \frac{1}{e}$ – which suggests that the eventual proof should rely on other value of λ. This problem is left for future research.

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A Proof of Lemma 3

We now proceed to the proof of Lemma 3. First, let us introduce $f(s) = p^s + ps - 2p$, so that

$$D(s) = \prod_{i=0}^{\infty} f(s-i)p^{-(s-i)}.$$

Observe that $f(s)$ has only two roots, given by Lambert function W, which is the inverse of function xe^x: $W^{-1}(x) = xe^x$. There are only two roots for real numbers which corresponds to two branches W_0 and W_{-1} of the function W. Therefore, any chosen $c < 0$ is smaller than the roots of $f(s)$ and the distance between c and any root is at least 1.

▶ **Lemma 8.** *For all $0 < \varepsilon < 1$ and $c < 0$ it holds that $\min_{\mathrm{Re}(s)=c} |f(s)| \geq \Theta(p^{(1-\varepsilon)(c-1)}) > 0$.*

Proof. We have $f'(s) = p^s \ln(p) + p$ and $f''(s) = p^s \ln^2(p)$.

Let us consider a complex disk of radius $R = p^{-\varepsilon(c-1)}$ $(R < 1)$ centered on s. For $\theta \in (0, 2\pi)$ by virtue of Taylor-Young theorem we have:

$$f(s + Re^{i\theta}) = f(s) + f'(s)e^{i\theta}R + \int_0^R f''(s + \rho e^{i\theta})e^{2i\theta}\rho \,\mathrm{d}\rho.$$

Now observe that

$$\begin{aligned}
\left|\int_0^R f''(s+\rho e^{i\theta})e^{2i\theta}\rho\,\mathrm{d}\rho\right| &= \left|p^s \ln^2(p) e^{2i\theta}\int_0^R p^{\rho\exp(i\theta)}\rho\,\mathrm{d}\rho\right| \\
&= \left|p^s\left(e^{R\exp(i\theta)\ln(p)}\left[R\exp(i\theta)\ln(p) - 1\right] + 1\right)\right| \\
&= O\left(\left|p^s R^2 e^{2i\theta}\right|\right) = O\left(p^c R^2\right),
\end{aligned}$$

where the last line follows from the fact that asymptotically $e^x(x-1)+1 = O(x^2)$ for $x \to 0$.

When θ varies the quantity $f'(s)e^{i\theta}R$ describes a circle of radius $|f'(s)|R = (-p^c\ln(p) + O(p))R$ around $f(s)$. The error term bound implies that each point of $f(s + Re^{i\theta})$ is at distance $O(p^cR^2)$ of this circle. Thus the image by f of the disk with center s and radius R contains the disk of center $f(s)$ and radius

$$\begin{aligned}
R|f'(s)| - O(R^2p^c) &= -p^{-\varepsilon(c-1)}p^c\ln(p) - O(p^{1-\varepsilon(c-1)}) - O\left(p^{-2\varepsilon(c-1)}p^c\right) \\
&= p^{(1-\varepsilon)(c-1)}\left(-p\ln(p) - O(p^{1-c}) - O(p^{-\varepsilon(c-1)})\right) = \Theta(p^{(1-\varepsilon)(c-1)}).
\end{aligned}$$

The point $s = 0$ cannot be in this disk, otherwise the function $f(s)$ would have other roots than the expected ones, thus necessarily $|f(s)| \geq \Theta(p^{(1-\varepsilon)(c-1)})$. ◀

Let now $g(s) = p^{-s}f(s)$ so that

$$D(s) = \prod_{i=0}^{\infty} g(s-i).$$

▶ **Lemma 9.** *For t real and $c < 0$, the following inequality holds*

$$|g(c+it)| \geq |1 - p^{1-c}(2-c) - p^{1-c}|t||.$$

Proof. We have

$$\begin{aligned}
|g(c+it)| &= |p^{-c}f(c+it)| = |p^{it} + p^{1-c}(c-2) + p^{1-c}it| \\
&\geq ||p^{it}| - |p^{1-c}(c-2)| - |p^{1-c}it||.
\end{aligned}$$

But now observe that $|p^{it}| = 1$, which completes the proof. ◀

▶ **Lemma 10.** *For $c \in (-1, 0)$ and for all real number t outside any neighborhood of 0, for all $\varepsilon > 0$ it is true that* $\frac{1}{D(c+it)} = O(\exp\left(-(\log_p^2 |t|/2 + O(\log|t|)\right)$.

Proof. From Lemmas 8 and 9, it follows that:

$$|D(c+it)| \geq \prod_{k\geq 0} \max\{Bp^{-\varepsilon(1-c)}, \left|1 - (|t| + 2 + k - c)p^{k+1-c}\right|\}$$

For a given real number t, we denote $k(t)$ the largest integer k such that $(|t|+2+k-c)p^{k+1-c} > 1$, and we split the product at $k = k(t)$:

$$\begin{aligned} |D(c+it)| &\geq \prod_{k<k(t)} \left((|t| + 2 + k - c)\, p^{k+1-c} - 1\right) \\ &\qquad B'|t|^{-\epsilon} \prod_{k>k(t)} \left(1 - (|t| + 2 + k - c)\, p^{k+1-c}\right) \\ &\geq \left(\prod_{k<k(t)} \left(p^{k-k(t)} \left(1 - (k(t) - k)\, p^{k(t)+1-c}\right) - 1\right)\right) \\ &\qquad B'|t|^{-\epsilon} \prod_{k>k(t)} \left(1 - p^{k-k(t)} \left(1 - (k(t) - k)\, p^{k(t)-c}\right)\right) \end{aligned}$$

Now

$$\prod_{k>k(t)} \left(1 - p^{k-k(t)} \left(1 - (k(t) - k)\, p^{k(t)-c}\right)\right) \geq \prod_{k>0} (1 - p^k).$$

Furthermore $\prod_{k<k(t)} p^{k-k(t)} \geq p^{k(t)(k(t)-1)/2}$, thus

$$\prod_{k<k(t)} \left(p^{k-k(t)} \left(1 - (k(t) - k)\, p^{k(t)+1-c} - 1\right)\right) \geq p^{k(t)(k(t)-1)/2} \prod_{k>0} (1 - p^k).$$

Finally, $p^{-k(t)} = |t|p^{-c}$ and therefore

$$|D(c+it)| \geq p^{k(t)(k(t)-1)/2} B'|t|^{-\epsilon} \prod_{k>0} (1 - p^k)^2 = B'' \frac{|t|^{-\epsilon}}{(|t|p^{-c})^{(k(t)-1)/2}}.$$

We conclude, since $k(t) = c - \log_p |t|$. ◀

Notice that $D(c + it)$ tends to infinity when $|t| \to \infty$. To conclude the proof of Lemma 3 it is sufficient to observe that the function $1/D(s)$ for s is any compact set containing a neighborhood of $\mathrm{Re}(s)$ and away from the roots of $f(s)$ is naturally bounded by dominated convergence of the product.

Hidden Words Statistics for Large Patterns

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Abstract

We study here the so called *subsequence pattern matching* also known as *hidden pattern matching* in which one searches for a given pattern w of length m as a *subsequence* in a random text of length n. The quantity of interest is the number of occurrences of w as a subsequence (i.e., occurring in *not* necessarily consecutive text locations). This problem finds many applications from intrusion detection, to trace reconstruction, to deletion channel, and to DNA-based storage systems. In all of these applications, the pattern w is of variable length. To the best of our knowledge this problem was only tackled for a fixed length $m = O(1)$ [6]. In our main result Theorem 5 we prove that for $m = o(n^{1/3})$ the number of subsequence occurrences is normally distributed. In addition, in Theorem 6 we show that under some constraints on the structure of w the asymptotic normality can be extended to $m = o(\sqrt{n})$. For a special pattern w consisting of the same symbol, we indicate that for $m = o(n)$ the distribution of number of subsequences is either asymptotically normal or asymptotically log normal. We conjecture that this dichotomy is true for all patterns. We use Hoeffding's projection method for U-statistics to prove our findings.

2012 ACM Subject Classification Mathematics of computing → Probability and statistics

Keywords and phrases Hidden pattern matching, subsequences, probability, U-statistics, projection method

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.17

Funding *Svante Janson*: Supported by the Knut and Alice Wallenberg Foundation.
Wojciech Szpankowski: This work was supported by NSF Center for Science of Information (CSoI) Grant CCF-0939370, and in addition by NSF Grant CCF-1524312.

1 Introduction and Motivation

One of the most interesting and least studied problem in pattern matching is known as the *subsequence string matching* or the *hidden pattern matching* [11]. In this case, we search for a pattern $w = w_1w_2\cdots w_m$ of length m in the text $\Xi^n = \xi_1 \ldots \xi_n$ of length n as *subsequence*, that is, we are looking for indices $1 \le i_1 < i_2 < \cdots < i_m \le n$ such that $\xi_{i_1} = w_1, \xi_{i_2} = w_2, \ldots, \xi_{i_m} = w_m$. We say that w is *hidden* in the text Ξ^n. We do not put any constraints on the gaps $i_{j+1} - i_j$, so in language of [6] this is known as the *unconstrained* hidden pattern matching. The most interesting quantity of such a problem is the number of subsequence occurrences in the text generated by a random source. In this paper, we study the limiting distribution of this quantity when m, the length of the pattern, grows with n.

Hereafter, we assume that a memoryless source generates the text Ξ, that is, all symbols are generated independently with probability p_a for symbol $a \in \mathcal{A}$, where the alphabet $\mathcal{A}$ is assumed to be finite. We denote by $p_w = \prod_j p_{w_j}$ the probability of the pattern w. Our goal is to understand the probabilistic behavior, in particular, the limiting distribution of the number of subsequence occurrences that we denote by $Z := Z_\Xi(w)$. It is known that the behavior of Z depends on the order of magnitude of the pattern length m. For example,

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 17; pp. 17:1–17:15
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

for the *exact pattern matching* (i.e., the pattern w must occur as a *string* in consecutive positions of the text), the limiting distribution is normal for $m = O(1)$ (more precisely, when $np_w \to \infty$, hence up to $m = O(\log n)$), but it becomes a Pólya–Aeppli distribution when $np_w \to \lambda > 0$ for some constant λ, and finally (conditioned on being non-zero) it turns into a geometric distribution when $np_w \to 0$ [11] (see also [1]). We might expect a similar behaviour for the subsequence pattern matching. In [6] it was proved by analytic combinatoric methods that the number of subsequence occurrences, $Z_\Xi(w)$, is asymptotically normal when $m = O(1)$, and not much is known beyond this regime. (See also [2]. Asymptotic normality for fixed m follows also by general results for U-statistics [9].) However, in many applications – as discussed below – we need to consider patterns w whose lengths grow with n. In this paper, we prove two main results. In Theorem 5 we establish that for $m = o(n^{1/3})$ the number of subsequence occurrences is normally distributed. Furthermore, in Theorem 6 we show that under some constraints on the structure of w, the asymptotic normality can be extended to $m = o(\sqrt{n})$. Moreover, for the special pattern $w = a^m$ consisting of the same symbol repeated, we show in Theorem 4 that for $m = o(\sqrt{n})$, the distribution of number of occurrences is asymptotically normal, while for larger m (up to cn for some $c > 0$) it is asymptotically log-normal. We conjecture that this dichotomy is true for a large class of patterns.

Regarding methodology, unlike [6] we use here probabilistic tools. We first observe that Z can be represented as a U-statistic (see (2)). This suggests to apply the [9] projection method to prove asymptotic normality of Z for some large patterns. Indeed, we first decompose Z into a sum of orthogonal random variables with variances of decreasing order in n (for m not too large), and show that the variable of the largest variance converges to a normal distribution, proving our main results Theorems 5 and 6.

The hidden pattern matching problem, especially for large patterns, finds many applications from intrusion detection, to trace reconstruction, to deletion channel, to DNA-based storage systems [8, 5, 3, 11, 16]. Here we discuss below in some detail two of them, namely the deletion channel and the trace reconstruction problem.

A deletion channel [5, 3, 4, 13, 16, 17] with parameter d takes a binary sequence $\Xi^n = \xi_1 \cdots \xi_n$ where $\xi_i \in \mathcal{A}$ as input and deletes each symbol in the sequence independently with probability d. The output of such a channel is then a *subsequence* $\zeta = \zeta(x) = \xi_{i_1} ... \xi_{i_M}$ of Ξ, where M follows the binomial distribution $\mathrm{Binom}(n, (1 - d))$, and the indices $i_1, ..., i_M$ correspond to the bits that are *not* deleted. Despite significant effort [3, 13, 14, 16, 17] the mutual information between the input and output of the deletion channel and its capacity are still unknown. We hope to provide a more detailed characterization of the mutual information for memoryless sources using results of this and forthcoming papers. Indeed, it turns out that the mutual information $I(\Xi^n; \zeta(\Xi^n))$ can be exactly formulated as the problem of the subsequence pattern matching. In [5] it was proved that

$$I(\Xi^n;\zeta(\Xi^n))=\sum_w d^{n-|w|}(1-d)^{|w|}(\mathbb{E}[Z_{\Xi^n}(w)\log Z_{\Xi^n}(w)] - \mathbb{E}[Z_{\Xi^n}(w)]\log \mathbb{E}[Z_{\Xi^n}(w)]), \quad (1)$$

where the sum is over all binary sequences of length smaller than n and $Z_{\Xi^n}(w)$ is the number of subsequence occurrences of w in the text Ξ^n. As one can see, to find precise asymptotics of the mutual information we need to understand the probabilistic behavior of Z for $m \le n$ and typical w, which is our long term goal. The trace reconstruction problem [10, 15, 18] is related to the deletion channel problem since we are asking how many copies of the output deletion channel we need to see until we can reconstruct the input sequence with high probability.

2 Main Results

In this section we formulate precisely our problem and present our main results. Proofs are delayed till the next section.

2.1 Problem formulation and notation

We consider a random string $\Xi^n = \xi_1 \dots \xi_n$ of length n. We assume that $\xi_1, \xi_2, \dots$ are i.i.d. random letters from a finite alphabet $\mathcal{A}$; each letter ξ_i has the distribution $\mathbb{P}(\xi_i = a) = p_a$ where $a \in \mathcal{A}$, for some given vector $\mathbf{p} = (p_a)_{a\in\mathcal{A}}$; we assume $p_a > 0,\ a \in \mathcal{A}$.

Let $w = w_1 \cdots w_m$ be a fixed string of length m over the same alphabet $\mathcal{A}$. We assume $n \geq m$. Let $p_w := \prod_{j=1}^m p_{w_j}$, which is the probability that $\xi_1 \cdots \xi_m$ equals w.

Let $Z = Z_{n,w}(\xi_1 \cdots \xi_n)$ be the number of occurrences of w as a subsequence of $\xi_1 \cdots \xi_n$. For a set $\mathcal{S}$ (in our case $[n]$ or $[m]$) and $k \geq 0$, let $\binom{\mathcal{S}}{k}$ be the collection of sets $\alpha \subseteq \mathcal{S}$ with $|\alpha| = k$. Thus, $\bigl|\binom{\mathcal{S}}{k}\bigr| = \binom{|\mathcal{S}|}{k}$. For $k = 0$, $\binom{\mathcal{S}}{0}$ contains just the empty set $\emptyset$. For $k = 1$, we identify $\binom{\mathcal{S}}{1}$ and $\mathcal{S}$ in the obvious way. We write $\alpha \in \binom{[n]}{k}$ as $\{\alpha_1, \dots, \alpha_k\}$, where we assume that $\alpha_1 < \dots < \alpha_k$. Then

$$Z = \sum_{\alpha\in\binom{[n]}{m}} I_\alpha, \quad \text{where} \quad I_\alpha = \prod_{j=1}^m \mathbf{1}\{\xi_{\alpha_j} = w_j\}, \quad \alpha_1 < \ldots < \alpha_m. \tag{2}$$

▶ Remark 1. In the limit theorems, we are studying the asymptotic distribution of Z. We then assume that $n \to \infty$ and (usually) $m \to \infty$; we thus implicitly consider a sequence of words $w^{(n)}$ of lengths $m_n = |w^{(n)}|$. But for simplicity we do not show this in the notation.

We have $\mathbb{E}\, I_\alpha = p_w$ for every α. Hence,

$$\mathbb{E}\, Z = \sum_{\alpha\in\binom{[n]}{m}} \mathbb{E}\, I_\alpha = \binom{n}{m} p_w. \tag{3}$$

Further, let $Y_\alpha := p_w^{-1} I_\alpha$, so $\mathbb{E}\, Y_\alpha = 1$, and

$$Z^* := p_w^{-1} Z = \sum_{\alpha\in\binom{[n]}{m}} Y_\alpha, \tag{4}$$

so $\mathbb{E}\, Z^* = \binom{n}{m}$ and

$$Z^* - \mathbb{E}\, Z^* = p_w^{-1} Z - \binom{n}{m} = \sum_{\alpha\in\binom{[n]}{m}} (Y_\alpha - 1). \tag{5}$$

We also write $\|Y\|_p := \bigl(\mathbb{E}\, |Y|^p\bigr)^{1/p}$ for the L^p norm of a random variable Y, while $\|\mathbf{x}\|$ is the usual Euclidean norm of a vector $\mathbf{x}$ in some $\mathbb{R}^m$. C denotes constants that may be different at different occurrences; they may depend on the alphabet $\mathcal{A}$ and $(p_a)_{a\in\mathcal{A}}$, but not on n, m or w. Finally, $\xrightarrow{\mathrm{d}}$ and $\xrightarrow{\mathrm{p}}$ mean convergence in distribution and probability, respectively.

We are now ready to present our main results regarding the limiting distribution of Z, the number of subsequence $w = a_1, \dots a_m$ occurrences when $m \to \infty$. We start with a simple example, namely, $w = a^m = a \cdots a$ for some $a \in \mathcal{A}$, and show that depending on whether $m = o(\sqrt{n})$ or not the number of subsequences will follow asymptotically either the normal distribution or the log-normal distribution.

Before we present our results we consider asymptotically normal and log-normal distributions in general, and discuss their relation.

2.2 Asymptotic normality and log-normality

If X_n is a sequence of random variables and a_n and b_n are sequences of real numbers, with $b_n > 0$, then $X_n \sim \mathrm{AsN}(a_n, b_n)$ means that

$$\frac{X_n - a_n}{\sqrt{b_n}} \xrightarrow{\mathrm{d}} N(0,1). \tag{6}$$

We say that X_n is *asymptotically normal* if $X_n \sim \mathrm{AsN}(a_n, b_n)$ for some a_n and b_n, and *asymptotically log-normal* if $\ln X_n \sim \mathrm{AsN}(a_n, b_n)$ for some a_n and b_n (this assumes $X_n \geq 0$). Note that these notions are equivalent when the asymptotic variance b_n is small, as made precise by the following lemma.

▶ **Lemma 2.** *If $b_n \to 0$, and a_n are arbitrary, then*

$$\ln X_n \sim \mathrm{AsN}(a_n, b_n) \iff X_n \sim \mathrm{AsN}(e^{a_n}, b_n e^{2a_n}). \tag{7}$$

Proof. By replacing X_n by X_n/e^{a_n}, we may assume that $a_n = 0$. If $\ln X_n \sim \mathrm{AsN}(0, b_n)$ with $b_n \to 0$, then $\ln X_n \xrightarrow{\mathrm{p}} 0$, and thus $X_n \xrightarrow{\mathrm{p}} 1$. It follows that $\ln X_n/(X_n - 1) \xrightarrow{\mathrm{p}} 1$ (with $0/0 := 1$), and thus

$$\frac{X_n - 1}{b_n^{1/2}} = \frac{X_n - 1}{\ln X_n} \frac{\ln X_n}{b_n^{1/2}} \xrightarrow{\mathrm{d}} N(0,1), \tag{8}$$

and thus $X_n \sim \mathrm{AsN}(1, b_n)$. The converse is proved by the same argument. ◀

▶ Remark 3. Lemma 2 is best possible. Suppose that $\ln X_n \sim \mathrm{AsN}(a_n, b_n)$. If $b_n \to b > 0$, then $\ln\bigl(X_n/e^{a_n}\bigr) = \ln X_n - a_n \xrightarrow{\mathrm{d}} N(0, b)$, and thus

$$X_n/e^{a_n} \xrightarrow{\mathrm{d}} e^{\zeta_b}, \qquad \zeta_b \sim N(0,b). \tag{9}$$

In this case (and only in this case), X_n thus converges in distribution, after scaling, to a log-normal distribution. If $b_n \to \infty$, then no linear scaling of X_n can converge in distribution to a non-degenerate limit, as is easily seen.

2.3 A simple example

We consider first a simple example where the asymptotic distribution can be found easily by explicit calculations. Fix $a \in \mathcal{A}$ and let $w = a^m = a \cdots a$, a string with m identical letters. Then, if $N = N_a$ is the number of occurrences of a in $\xi_1 \cdots \xi_n$, then

$$Z = \binom{N_a}{m}. \tag{10}$$

We will show that Z is asymptotically normal if m is small, and log-normal for larger m.

▶ **Theorem 4.** *Suppose that $m < np_a$, with $np_a - m \gg n^{1/2}$.*

(i) *Then*

$$\ln Z \sim \mathrm{AsN}\Bigl(\ln \binom{np_a}{m}, n\Bigl|\ln\Bigl(1 - \frac{m}{np_a}\Bigr)\Bigr|^2 p_a(1-p_a)\Bigr). \tag{11}$$

(ii) *In particular, if $m = o(n)$, then*

$$\ln Z \sim \mathrm{AsN}\Bigl(\ln \binom{np_a}{m}, \bigl(p_a^{-1} - 1\bigr)\frac{m^2}{n}\Bigr). \tag{12}$$

(iii) *If $m = o(n^{1/2})$, then this implies*

$$Z/\mathbb{E}\,Z \sim \mathrm{AsN}\Big(1, (p_a^{-1}-1)\frac{m^2}{n}\Big), \tag{13}$$

and thus

$$Z \sim \mathrm{AsN}\Big(\mathbb{E}\,Z, (p_a^{-1}-1)\frac{m^2}{n}(\mathbb{E}\,Z)^2\Big). \tag{14}$$

Proof. (i) We have $N_a \sim \mathrm{Bin}(n, p_a)$. Define $Y := N_a - np_a$. Then, by the Central Limit Theorem,

$$Y \sim \mathrm{AsN}\big(0, np_a(1-p_a)\big). \tag{15}$$

By (10), we have

$$\begin{aligned}
\ln Z - \ln\binom{np_a}{m} &= \ln\binom{np_a+Y}{m} - \ln\binom{np_a}{m} \\
&= \ln\Gamma(np_a+Y+1) - \ln\Gamma(np_a+Y-m+1) - \ln m! \\
&\quad - \big(\ln\Gamma(np_a+1) - \ln\Gamma(np_a-m+1) - \ln m!\big) \\
&= \int_{y=0}^{Y}\int_{x=-m}^{0} (\ln\Gamma)''(np_a+x+y+1)\,\mathrm{d}x\,\mathrm{d}y.
\end{aligned} \tag{16}$$

We fix a sequence $\omega_n \to \infty$ such that $np_a - m \gg \omega_n \gg n^{1/2}$; this is possible by the assumption. Note that (15) implies that $Y/\omega_n \xrightarrow{\mathrm{p}} 0$, and thus $\mathbb{P}(|Y| \le \omega_n) \to 1$. We may thus in the sequel assume $|Y| \le \omega_n$. We assume also that n is so large that $np_a - m \ge 2\omega_n > 0$.

Stirling's formula implies, by taking the logarithm and differentiating twice (in the complex half-plane $\mathrm{Re}\,z > \frac{1}{2}$, say)

$$(\ln\Gamma)''(x) = \frac{1}{x} + O\Big(\frac{1}{x^2}\Big) = \frac{1}{x}\Big(1 + O\Big(\frac{1}{x}\Big)\Big), \qquad x \ge 1. \tag{17}$$

Consequently, (16) yields, noting the assumptions just made imply $|Y| \le \omega_n \le \frac{1}{2}(np_a - m)$,

$$\begin{aligned}
\ln Z - \ln\binom{np_a}{m} &= \int_{y=0}^{Y}\int_{x=-m}^{0} \frac{1}{np_a+x+y+1}\Big(1+O\Big(\frac{1}{np_a-m}\Big)\Big)\,\mathrm{d}x\,\mathrm{d}y \\
&= \int_{y=0}^{Y}\int_{x=-m}^{0} \frac{1}{np_a+x}\Big(1+O\Big(\frac{\omega_n}{np_a-m}\Big)\Big)\,\mathrm{d}x\,\mathrm{d}y \\
&= \Big(1+O\Big(\frac{\omega_n}{np_a-m}\Big)\Big)Y\int_{x=-m}^{0}\frac{1}{np_a+x}\,\mathrm{d}x \\
&= \big(1+o(1)\big)Y\ln\frac{np_a}{np_a-m}.
\end{aligned} \tag{18}$$

Consequently, using also (15), we obtain

$$\frac{\ln Z - \ln\binom{np_a}{m}}{n^{1/2}\big|\ln\big(1-\frac{m}{np_a}\big)\big|} = \big(1+o_{\mathrm{p}}(1)\big)\frac{Y}{n^{1/2}} \xrightarrow{\mathrm{d}} N\big(0, p_a(1-p_a)\big), \tag{19}$$

which is equivalent to (11).

(ii) If $m = o(n)$, then $\left|\ln\left(1 - \frac{m}{np_a}\right)\right| \sim \frac{m}{np_a}$, and (12) follows.
(iii) If $m = o(n^{1/2})$, then (ii) applies, so (12) holds; hence Lemma 2 implies

$$Z/\binom{np_a}{m} \sim \mathrm{AsN}\Big(1, (p_a^{-1} - 1)\frac{m^2}{n}\Big). \tag{20}$$

Furthermore,

$$\mathbb{E}\, Z = \binom{n}{m} p_a^m = \frac{n^m e^{O(m^2/n)}}{m!} p_a^m \sim \frac{n^m}{m!} p_a^m \tag{21}$$

and, similarly, $\binom{np_a}{m} \sim \frac{n^m p_a^m}{m!}$. Hence, $\mathbb{E}\, Z \sim \binom{np_a}{m}$ and (13) follows from (20); (14) is an immediate consequence. ◀

2.4 General results

We now present our main results. However, first we discuss the road map of our approach. First, we observe that the representation (2) shows that Z can be viewed as a U-statistic. For convenience, we consider Z^* in (4), which differs from Z by a constant factor only, and show in (41) that $Z^* - \mathbb{E}\, Z^*$ can be decomposed into a sum $\sum_{\ell=1}^m V_\ell$ of orthogonal random variables V_ℓ such that, when m is not too large, $\mathrm{Var}\big(\sum_{\ell=2}^m V_\ell\big) = o(\mathrm{Var}\, V_1)$. Next, in Lemma 11 we prove that V_1 appropriately normalized converges to the standard normal distribution. This will allow us to conclude the asymptotic normality of Z.

In this paper, we only consider the region $m = o\big(n^{1/2}\big)$. First, for $m = o\big(n^{1/3}\big)$ we claim that the number of subsequence occurrences always is asymptotically normal.

▶ **Theorem 5.** *If $m = o\big(n^{1/3}\big)$, then*

$$Z \sim \mathrm{AsN}\Big(\binom{n}{m} p_w, \sigma_1^2 p_w^2\Big), \tag{22}$$

where

$$\sigma_1^2 = \sum_{i=1}^n \sum_{a\in\mathcal{A}} p_a^{-1} \left(\sum_{j:\ w_j = a} \binom{i-1}{j-1}\binom{n-i}{m-j} \right)^2 - n\binom{n-1}{m-1}^2. \tag{23}$$

Furthermore, $\mathbb{E}\, Z = \binom{n}{m} p_w$ and $\mathrm{Var}\, Z \sim p_w^2 \sigma_1^2$.

In the second main result, we restrict the patterns w to such that are not typical for the random text; however, we will allow $m = o\big(n^{1/2}\big)$.

▶ **Theorem 6.** *Let $\mathbf{q} = (q_a)_{a\in\mathcal{A}}$ be the proportions of the letters in w, i.e., $q_a := \frac{1}{m}\sum_{j=1}^m \mathbf{1}\{w_j = a\}$. Suppose that $\liminf_{n\to\infty} \|\mathbf{q} - \mathbf{p}\| > 0$. If further $m = o\big(n^{1/2}\big)$, then the asymptotic normality (22) holds.*

3 Analysis and Proofs

In this section we will prove our main results. We start with some preliminaries.

3.1 Preliminaries and more notation

Let, for $a \in \mathcal{A}$,

$$\varphi_a(x) := p_a^{-1}\mathbf{1}\{x = a\} - 1. \tag{24}$$

Thus, letting ξ be any random variable with the distribution of ξ_i,

$$\mathbb{E}\,\varphi_a(\xi) = 0, \qquad a \in \mathcal{A}. \tag{25}$$

Let $p_* := \min_a p_a$ and

$$B := p_*^{-1} - 1. \tag{26}$$

▶ **Lemma 7.** *Let φ_a and B be as above.*

(i) *For every $a \in \mathcal{A}$,*

$$\mathbb{E}\big[\varphi_a(\xi)^2\big] = p_a^{-1} - 1 \le B. \tag{27}$$

(ii) *For some $c_1 > 0$ and every $a \in \mathcal{A}$,*

$$\|\varphi_a(\xi)\|_2 = \big(p_a^{-1} - 1\big)^{1/2} \ge c_1. \tag{28}$$

(iii) *For any vector $\mathbf{r} = (r_a)_{a\in\mathcal{A}}$ with $\sum_a r_a = 1$,*

$$\Big\|\sum_{a\in\mathcal{A}} r_a\varphi_a(\xi)\Big\|_2 \ge \|\mathbf{r}-\mathbf{p}\| := \Big(\sum_{a\in\mathcal{A}} |r_\alpha - p_\alpha|^2\Big)^{1/2}. \tag{29}$$

Proof. The definition (24) yields

$$\mathbb{E}\big[\varphi_a(\xi)^2\big] = p_a^{-2}\operatorname{Var}\big[\mathbf{1}\{\xi = a\}\big] = p_a^{-2}p_a(1-p_a) = p_a^{-1} - 1. \tag{30}$$

Hence, (27) and (28) follow, with B given by (26).

Finally, for every $x \in \mathcal{A}$, by (24) again,

$$\sum_{a\in\mathcal{A}} r_a\varphi_a(x) = r_x p_x^{-1} - \sum_{a\in\mathcal{A}} r_a = r_x/p_x - 1 \tag{31}$$

and thus

$$\mathbb{E}\Big(\sum_{a\in\mathcal{A}} r_a\varphi_a(\xi)\Big)^2 = \sum_{a\in\mathcal{A}} p_a\big(r_a/p_a - 1\big)^2 = \sum_{a\in\mathcal{A}} p_a^{-1}\big(r_a - p_a\big)^2 \tag{32}$$

and (29) follows. ◀

3.2 A decomposition

The representation (2) shows that Z is a special case of a U-statistic. For fixed m, the general theory of [9] applies and yields asymptotic normality. (Cf. [12, Section 4] for a related problem.) For $m \to \infty$ (our main interest), we can still use the orthogonal decomposition of [9], which in our case takes the following form.

By the definitions in Section 2.1 and (24),

$$Y_\alpha = \prod_{j=1}^{m}\big(p_{w_j}^{-1}\mathbf{1}\{\xi_{\alpha_j} = w_j\}\big) = \prod_{j=1}^{m}\big(\varphi_{w_j}(\xi_{\alpha_j}) + 1\big). \tag{33}$$

By multiplying out this product, we obtain

$$Y_\alpha = \sum_{\gamma\subseteq[m]}\prod_{j\in\gamma}\varphi_{w_j}(\xi_{\alpha_j}). \tag{34}$$

Hence,

$$Z^* = \sum_{\alpha\in\binom{[n]}{m}} Y_\alpha = \sum_{\alpha\in\binom{[n]}{m}} \sum_{\gamma\subseteq[m]} \prod_{j\in\gamma} \varphi_{w_j}(\xi_{\alpha_j}) = \sum_{\alpha\in\binom{[n]}{m}} \sum_{\gamma\subseteq[m]} \prod_{k=1}^{|\gamma|} \varphi_{w_{\gamma_k}}(\xi_{\alpha_{\gamma_k}}). \tag{35}$$

We rearrange this sum. First, let $\ell := |\gamma| \in [m]$, and consider all terms with a given ℓ. For each α and γ, with $|\gamma| = \ell$, let

$$\alpha_\gamma := \{\alpha_{\gamma_1}, \dots, \alpha_{\gamma_\ell}\} \in \binom{[n]}{\ell}. \tag{36}$$

For given $\gamma \in \binom{[m]}{\ell}$ and $\beta \in \binom{[n]}{\ell}$, the number of $\alpha \in \binom{[n]}{m}$ such that $\alpha_\gamma = \beta$ equals the number of ways to choose, for each $k \in [\ell+1]$, $\gamma_k - \gamma_{k-1} - 1$ elements of α in a gap of length $\beta_k - \beta_{k-1} - 1$, where we define $\beta_0 = \gamma_0 = 0$ and $\beta_{\ell+1} = n+1$, $\gamma_{\ell+1} = m+1$; this number is

$$c(\beta,\gamma) := \prod_{k=1}^{\ell+1} \binom{\beta_k - \beta_{k-1} - 1}{\gamma_k - \gamma_{k-1} - 1}. \tag{37}$$

Consequently, combining the terms in (35) with the same α_γ,

$$Z^* = \sum_{\ell=0}^{m} \sum_{\gamma\in\binom{[m]}{\ell}} \sum_{\beta\in\binom{[n]}{\ell}} c(\beta,\gamma) \prod_{k=1}^{\ell} \varphi_{w_{\gamma_k}}(\xi_{\beta_k}). \tag{38}$$

We define, for $0 \le \ell \le m$ and $\beta \in \binom{[n]}{\ell}$,

$$V_{\ell,\beta} := \sum_{\gamma\in\binom{[m]}{\ell}} c(\beta,\gamma) \prod_{k=1}^{\ell} \varphi_{w_{\gamma_k}}(\xi_{\beta_k}) \tag{39}$$

and

$$V_\ell := \sum_{\beta\in\binom{[n]}{\ell}} V_{\ell,\beta}. \tag{40}$$

Thus (38) yields the decomposition

$$Z^* = \sum_{\ell=0}^{m} V_\ell. \tag{41}$$

For $\ell = 0$, $\binom{[n]}{0}$ contains only the empty set $\emptyset$, and

$$V_0 = V_{0,\emptyset} = \binom{n}{m} = \mathbb{E}\, Z^*. \tag{42}$$

Furthermore, note that two summands in (38) with different β are orthogonal, as a consequence of (25) and independence of different ξ_i. Consequently, the variables $V_{\ell,\beta}$ ($\ell \in [m]$, $\beta \in \binom{[n]}{\ell}$) are orthogonal, and hence the variables V_ℓ ($\ell = 0, \dots, m$) are orthogonal.

Let

$$\sigma_\ell^2 := \operatorname{Var}(V_\ell) = \mathbb{E}\, V_\ell^2 = \sum_{\beta\in\binom{[m]}{\ell}} \mathbb{E}\, V_{\ell,\beta}^2, \qquad 1 \le \ell \le m. \tag{43}$$

Note also that by the combinatorial definition of $c(\beta,\gamma)$ given before (37), we see that

$$\sum_{\beta\in\binom{[n]}{\ell}} c(\beta,\gamma) = \binom{n}{m}, \tag{44}$$

since this is just the number of $\alpha \in \binom{[n]}{m}$, and

$$\sum_{\gamma\in\binom{[m]}{\ell}} c(\beta,\gamma) = \binom{n-\ell}{m-\ell}, \tag{45}$$

since this sum is the total number of ways to choose $m-\ell$ elements of the $n-\ell$ elements of α in the gaps.

3.3 The projection method

We use the projection method used by [9] to prove asymptotic normality for U-statistics. Translated to the present setting, the idea of the projection method is to approximate $Z^* - \mathbb{E}\,Z^* = Z^* - V_0$ by V_1, thus ignoring all terms with $\ell \geq 2$ in the sum in (41). In order to do this, we estimate variances.

First, by (27) and the independence of the ξ_i,

$$\Big\|\prod_{k=1}^{\ell} \varphi_{w_{\gamma_k}}(\xi_{\beta_k})\Big\|_2 = \Big(\prod_{k=1}^{\ell} \mathbb{E}\big|\varphi_{w_{\gamma_k}}(\xi_{\beta_k})\big|^2\Big)^{1/2} \leq B^{\ell/2}. \tag{46}$$

By Minkowski's inequality, (39), (46) and (45),

$$\|V_{\ell,\beta}\|_2 \leq \sum_{\gamma\in\binom{[m]}{\ell}} c(\beta,\gamma) B^{\ell/2} = B^{\ell/2}\binom{n-\ell}{m-\ell} \tag{47}$$

or, equivalently,

$$\mathbb{E}\,V_{\ell,\beta}^2 \leq B^{\ell}\binom{n-\ell}{m-\ell}^2. \tag{48}$$

This leads to the following estimates.

▶ **Lemma 8.** *For $1 \leq \ell \leq m$,*

$$\sigma_\ell^2 := \mathbb{E}\,V_\ell^2 \leq \widehat{\sigma}_\ell^2 := B^\ell\binom{n}{\ell}\binom{n-\ell}{m-\ell}^2. \tag{49}$$

Proof. The definition of V_ℓ in (40) and (48) yield, since the summands $V_{\ell,\beta}$ are orthogonal,

$$\sigma_\ell^2 := \mathbb{E}\,V_\ell^2 = \sum_{\beta\in\binom{[n]}{\ell}} \mathbb{E}\,V_{\ell,\beta}^2 \leq \binom{n}{\ell}B^\ell\binom{n-\ell}{m-\ell}^2, \tag{50}$$

as needed. ◀

Note that, for $1 \leq \ell < m$,

$$\frac{\widehat{\sigma}_{\ell+1}^2}{\widehat{\sigma}_\ell^2} = B\frac{\binom{n}{\ell+1}\binom{n-\ell-1}{m-\ell-1}^2}{\binom{n}{\ell}\binom{n-\ell}{m-\ell}^2} = B\frac{n-\ell}{\ell+1}\Big(\frac{m-\ell}{n-\ell}\Big)^2 \leq B\frac{m^2}{(\ell+1)n}. \tag{51}$$

▶ **Lemma 9.** *If $m \le B^{-1/2}n^{1/2}$, then*

$$\operatorname{Var}\bigl(Z^* - V_1\bigr) \le B^2 m^2 \binom{n-1}{m-1}^2. \tag{52}$$

Proof. By (51) and the assumption, for $1 \le \ell < m$,

$$\frac{\widehat{\sigma}_{\ell+1}^2}{\widehat{\sigma}_\ell^2} \le \frac{1}{\ell+1} \le \frac{1}{2}, \tag{53}$$

and thus, summing a geometric series,

$$\begin{aligned}\operatorname{Var}\bigl(Z^* - V_1\bigr) &= \sum_{\ell=2}^{m} \operatorname{Var}\bigl(V_\ell\bigr) \le \sum_{\ell=2}^{m} \widehat{\sigma}_\ell^2 \le \sum_{\ell=2}^{m} 2^{2-\ell}\widehat{\sigma}_2^2 \le 2\widehat{\sigma}_2^2 \\ &= B^2 n(n-1)\binom{n-2}{m-2}^2 \le B^2 m^2 \binom{n-1}{m-1}^2.\end{aligned} \tag{54}$$

◀

3.4 The first term V_1

For $\ell = 1$, we identify $\binom{[n]}{\ell}$ and $[n]$, and we write $V_{1,i} := V_{1,\{i\}}$. Note that, by (37),

$$c(i,j) := c\bigl(\{i\},\{j\}\bigr) = \binom{i-1}{j-1}\binom{n-i}{m-j}. \tag{55}$$

Thus (40) and (39) become

$$V_1 = \sum_{i=1}^{n} V_{1,i} \tag{56}$$

with, using (55),

$$V_{1,i} = \sum_{j=1}^{m} c(i,j)\varphi_{w_j}(\xi_i) = \sum_{j=1}^{m} \binom{i-1}{j-1}\binom{n-i}{m-j}\varphi_{w_j}(\xi_i). \tag{57}$$

Note that $V_{1,i}$ is a function of ξ_i, and thus the random variables $V_{1,i}$ are independent. Furthermore, (25) implies $\mathbb{E}\,V_{1,i} = 0$. Let $\tau_i^2 := \operatorname{Var} V_{1,i} = \mathbb{E}\,V_{1,i}^2$. Then, see (43),

$$\sigma_1^2 = \operatorname{Var} V_1 = \sum_{i=1}^{n} \operatorname{Var} V_{1,i} = \sum_{i=1}^{n} \tau_i^2. \tag{58}$$

Observe that it follows from (57) and (24) that

$$\tau_i^2 = \sum_{a\in\mathcal{A}} p_a^{-1}\left(\sum_{j:\ w_j=a} \binom{i-1}{j-1}\binom{n-i}{m-j}\right)^2 - \binom{n-1}{m-1}^2. \tag{59}$$

Taking $\ell = 1$ in (48) yields the upper bound

$$\tau_i^2 = \mathbb{E}\,V_{1,i}^2 \le B\binom{n-1}{m-1}^2, \qquad i \in [n]. \tag{60}$$

Summing over i, or using (49), we obtain

$$\sigma_1^2 := \mathbb{E}\, V_1^2 \leq \widehat{\sigma}_1^2 := Bn\binom{n-1}{m-1}^2. \tag{61}$$

We notice that the upper bound is achievable. Indeed, for $w = a \cdots a$, by (59) and (58),

$$\tau_i^2 = (p_a^{-1} - 1)\binom{n-1}{m-1}^2, \qquad \sigma_1^2 = n(p_a^{-1} - 1)\binom{n-1}{m-1}^2. \tag{62}$$

We show also a general lower bound.

▶ **Lemma 10.** *There exists $c, c' > 0$ such that*

$$\sigma_1^2 \geq \frac{c}{m}\widehat{\sigma}_1^2 = c'\frac{n}{m}\binom{n-1}{m-1}^2. \tag{63}$$

Proof. We consider the first term in the sum in (57) separately, and write

$$V_{1,i} = c(i,1)\varphi_{w_1}(\xi_i) + V'_{1,i}, \tag{64}$$

where

$$V'_{1,i} := \sum_{j=2}^{m} c(i,j)\varphi_{w_j}(\xi_i). \tag{65}$$

We have, by (55), $c(i,1) = \binom{n-i}{m-1}$. Consequently, for any $i \in [n]$,

$$\begin{aligned}\frac{c(i,1)}{c(1,1)} &= \frac{\binom{n-i}{m-1}}{\binom{n-1}{m-1}} = \frac{\prod_{k=0}^{m-2}(n-i-k)}{\prod_{k=0}^{m-2}(n-1-k)} = \prod_{k=0}^{m-2}\Bigl(1 - \frac{i-1}{n-1-k}\Bigr) \\ &\geq 1 - \sum_{k=0}^{m-2}\frac{i-1}{n-1-k} \geq 1 - \frac{m(i-1)}{n-m+1}. \end{aligned} \tag{66}$$

Let $\delta \leq 1/4$ be a fixed small positive number, chosen later. Assume that $i \leq 1 + \delta n/m$. In particular, either $i = 1$ or $m \leq m(i-1) \leq \delta n < n/2$, and thus (66) implies

$$\frac{c(i,1)}{c(1,1)} \geq 1 - \frac{m(i-1)}{n-m} \geq 1 - \frac{\delta n}{n/2} = 1 - 2\delta. \tag{67}$$

By (45), (67) implies

$$\sum_{j=2}^{m} c(i,j) = \binom{n-1}{m-1} - c(i,1) = c(1,1) - c(i,1) \leq 2\delta c(1,1). \tag{68}$$

Hence, by (65), Minkowski's inequality and (27), cf. (47),

$$\bigl\|V'_{1,i}\bigr\|_2 \leq \sum_{j=2}^{m} c(i,j)\bigl\|\varphi_{w_j}(\xi_i)\bigr\|_2 \leq \sum_{j=2}^{m} c(i,j)B^{1/2} \leq 2\delta B^{1/2}c(1,1). \tag{69}$$

Furthermore, (28) and (67) yield

$$\bigl\|c(i,1)\varphi_{w_1}(\xi_i)\bigr\|_2 \geq c(i,1)c_1 \geq c_1(1-2\delta)c(1,1) \geq \tfrac{1}{2}c_1 c(1,1). \tag{70}$$

Finally, (64) and the triangle inequality yield, using (70) and (69),

$$\|V_{1,i}\|_2 \geq \|c(i,1)\varphi_{w_1}(\xi_i)\|_2 - \|V'_{1,i}\|_2 \geq \bigl(\tfrac{1}{2}c_1 - 2\delta B^{1/2}\bigr)c(1,1). \tag{71}$$

We now choose $\delta := c_1/(8B^{1/2})$, and find that for some $c_2 > 0$,

$$\tau_i^2 := \|V_{1,i}\|_2^2 \geq c_2 c(1,1)^2, \qquad i \leq 1 + \delta n/m. \tag{72}$$

Consequently, by (58),

$$\sigma_1^2 = \sum_{i=1}^{n} \tau_i^2 \geq \frac{\delta n}{m} c_2 c(1,1)^2 = c_3 \frac{n}{m} \binom{n-1}{m-1}^2. \tag{73}$$

This proves (63), with $c' := c_3$ and $c = c'/B$. ◀

The next lemma is proved in the Appendix in which we verify Lyapunov's condition to prove asymptotic normality of V_1.

▶ **Lemma 11.** *Suppose that $m = o(n)$. Then V_1 is asymptotically normal:*

$$V_1/\sigma_1 \xrightarrow{\mathrm{d}} N(0,1). \tag{74}$$

3.5 Proofs of Theorem 5 and 6

We next prove a general theorem showing asymptotic normality under some conditions.

▶ **Theorem 12.** *Suppose that $n \to \infty$ and that*

$$m^2 \binom{n-1}{m-1}^2 = o\bigl(\sigma_1^2\bigr). \tag{75}$$

Then

$$\operatorname{Var} Z = p_w^2 \operatorname{Var} Z^* \sim p_w^2 \sigma_1^2 \tag{76}$$

and

$$\frac{Z^* - \mathbb{E} Z^*}{\sigma_1} \xrightarrow{\mathrm{d}} N(0,1), \tag{77}$$

$$\frac{Z - \mathbb{E} Z}{(\operatorname{Var} Z)^{1/2}} = \frac{Z^* - \mathbb{E} Z^*}{(\operatorname{Var} Z^*)^{1/2}} \xrightarrow{\mathrm{d}} N(0,1). \tag{78}$$

Proof. By Lemma 9 and (75),

$$\operatorname{Var}\Bigl(\frac{Z^* - V_1}{\sigma_1}\Bigr) = \frac{\operatorname{Var}(Z^* - V_1)}{\sigma_1^2} \leq B^2 \frac{m^2 \binom{n-1}{m-1}^2}{\sigma_1^2} = o(1). \tag{79}$$

Hence, recalling $\mathbb{E} V_1 = 0$,

$$\frac{Z^* - \mathbb{E} Z^* - V_1}{\sigma_1} \xrightarrow{\mathrm{p}} 0. \tag{80}$$

Combining (74) and (80), we obtain (77).

Furthermore, by (79), and since the terms in (41) are orthogonal,

$$\operatorname{Var} Z^* = \operatorname{Var} V_1 + \operatorname{Var}\bigl(Z^* - V_1\bigr) = \sigma_1^2 + o(\sigma_1^2) \sim \sigma_1^2, \tag{81}$$

which yields (76), and also shows that we may replace σ_1 by $(\operatorname{Var} Z^*)^{1/2}$ in (77), which yields (78); the equality in (78) is a trivial consequence of (4). ◀

Now we are ready to prove our main results.

Proof of Theorem 5. By Lemma 10,

$$\frac{m^2\binom{n-1}{m-1}^2}{\sigma_1^2} \leq C\frac{m^3}{n} = o(1). \tag{82}$$

Thus (75) holds, and the result follows by Theorem 12 together with (3) and (4). ◀

Recall that in Theorem 6, the range of m is improved, assuming that w is *not* typical for the random source with probabilities $\mathbf{p} = (p_a)_{a\in\mathcal{A}}$ that we consider.

Proof of Theorem 6. By Theorem 12, with (75) verified by Lemma 13 below. ◀

▶ **Lemma 13.** *Let* $\mathbf{q} = (q_a)_{a\in\mathcal{A}}$ *be the proportions of the letters in* w*. Then*

$$\sigma_1^2 \geq \frac{m^2}{n}\binom{n}{m}^2 \|\mathbf{q}-\mathbf{p}\|^2 = n\binom{n-1}{m-1}^2 \|\mathbf{q}-\mathbf{p}\|^2. \tag{83}$$

Proof. Let

$$\psi_i(x) := \sum_{j=1}^{m} c(i,j)\varphi_{w_j}(x). \tag{84}$$

Thus (57) is $V_{1,i} = \psi_i(\xi_i)$, and (58) is, since $\mathbb{E}\,\psi_i(\xi) = 0$,

$$\sigma_1^2 = \operatorname{Var} V_1 = \sum_{i=1}^{n} \mathbb{E}\big[\psi_i(\xi_i)^2\big] = \mathbb{E}\sum_{i=1}^{n} \psi_i(\xi)^2. \tag{85}$$

Hence, by the Cauchy–Schwarz inequality,

$$n\sigma_1^2 = n\,\mathbb{E}\sum_{i=1}^{n}\psi_i(\xi)^2 \geq \mathbb{E}\Big(\sum_{i=1}^{n}\psi_i(\xi)\Big)^2. \tag{86}$$

Furthermore, by (84) and (44)

$$\sum_{i=1}^{n}\psi_i(x) = \sum_{i=1}^{n}\sum_{j=1}^{m} c(i,j)\varphi_{w_j}(x) = \sum_{j=1}^{m}\binom{n}{m}\varphi_{w_j}(x) = \binom{n}{m}\sum_{a\in\mathcal{A}} mq_a\varphi_a(x). \tag{87}$$

Hence, (29) yields

$$\Big\|\sum_{i=1}^{n}\psi_i(\xi)\Big\|_2 = m\binom{n}{m}\Big\|\sum_{a\in\mathcal{A}} q_a\varphi_a(\xi)\Big\|_2 \geq m\binom{n}{m}\|\mathbf{q}-\mathbf{p}\|. \tag{88}$$

Combining (86) and (88) yields (83). ◀

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A Appendix

A.1 Proof of Lemma 11

We show that the central limit theorem applies to the sum $V_1 = \sum_i V_{1,i}$ in (56). The terms $V_{1,i}$ are independent and have means $\mathbb{E}\, V_{1,i} = 0$. We verify Lyapunov's condition.

The random variable ξ is defined on some probability space $(\Omega, \mathcal{F}, P)$ and takes values in the finite set $\mathcal{A}$. Thus the linear space $\mathcal{V}$ of functions $\Omega \to \mathbb{R}$ of the form $f(\xi)$ has finite dimension $|\mathcal{A}|$. Moreover, every function in $\mathcal{V}$ is bounded. The L^2 and L^3 norms $\|\cdot\|_2$ and $\|\cdot\|_3$ are thus finite on $\mathcal{V}$, and are thus both norms on the finite-dimensional vector space $\mathcal{V}$; hence there exists a constant C such that for any function f,

$$\|f(\xi)\|_3 \le C\|f(\xi)\|_2. \tag{89}$$

In particular, since the definition (57) shows that $V_{1,i}$ is a function of $\xi_i \overset{\mathrm{d}}{=} \xi$,

$$\|V_{1,i}\|_3 \le C\|V_{1,i}\|_2 = C\tau_i, \qquad 1 \le i \le n. \tag{90}$$

Furthermore, by (60) and (63),

$$\frac{\max_i \tau_i^2}{\sigma_1^2} \le \frac{B\binom{n-1}{m-1}^2}{c'\frac{n}{m}\binom{n-1}{m-1}^2} = C\frac{m}{n} = o(1). \tag{91}$$

Consequently, using (90), (58) and (91),

$$\frac{\sum_{i=1}^{n} \mathbb{E}\,|V_{1,i}|^3}{\sigma_1^3} = \frac{\sum_{i=1}^{n} \|V_{1,i}\|_3^3}{\sigma_1^3} \le \frac{C\sum_{i=1}^{n} \tau_i^3}{\sigma_1^3} \le C\frac{\max_i \tau_i \sum_{i=1}^{n} \tau_i^2}{\sigma_1^3}$$
$$= C\frac{\max_i \tau_i}{\sigma_1} = o(1). \tag{92}$$

This shows the Lyapunov condition, and thus a standard form of the central limit theorem, [7, Theorem 7.2.4 or 7.6.2], yields (74).

The Giant Component and 2-Core in Sparse Random Outerplanar Graphs

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Abstract

Let $A(n,m)$ be a graph chosen uniformly at random from the class of all vertex-labelled outerplanar graphs with n vertices and m edges. We consider $A(n,m)$ in the sparse regime when $m = n/2 + s$ for $s = o(n)$. We show that with high probability the giant component in $A(n,m)$ emerges at $m = n/2 + O\left(n^{2/3}\right)$ and determine the typical order of the 2-core. In addition, we prove that if $s = \omega\left(n^{2/3}\right)$, with high probability every edge in $A(n,m)$ belongs to at most one cycle.

2012 ACM Subject Classification Mathematics of computing → Random graphs; Mathematics of computing → Generating functions

Keywords and phrases giant component, core, outerplanar graphs, singularity analysis

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.18

Related Version This extended abstract is based on the Master's thesis of Michael Missethan [16]. Detailed proofs of main and auxiliary results of this paper can be found in [16], `https://www.math.tugraz.at/~missethan/masters_thesis/arbeit.pdf`.

Funding *Mihyun Kang*: Research supported by the Austrian Science Fund (FWF): I3747, W1230.
Michael Missethan: Research supported by the Austrian Science Fund (FWF): W1230.

1 Introduction

1.1 Motivation

In 1959 Erdős and Rényi [5] introduced the so-called *Erdős-Rényi graph* $G(n,m)$, a graph chosen uniformly at random from the class of all vertex-labelled graphs on vertex set $\{1,\dots,n\}$ with $m = m(n)$ edges. Since then, the asymptotic behaviour of $G(n,m)$ was extensively studied (see e.g. [2, 8, 11]). In particular, it was investigated how the component structure of $G(n,m)$ changes, when $m = m(n)$ varies and whether there are ranges of m, where this change is very significant. Such dramatic changes are called *phase transitions*. For example, Erdős and Rényi [6] showed that the order (that is, the number of vertices) of the largest component in $G(n,m)$ changes drastically when $m \sim n/2$. Later Bollobás [1] and Łuczak [14] looked more closely at the critical range $m = n/2 + o(n)$.

Throughout the paper, we denote the components of a graph G by $H_1 = H_1(G), H_2 = H_2(G), \dots$ in such a way that $|H_i| \geq |H_j|$, whenever $i \leq j$, where $|H_i|$ is the number of vertices in H_i. In addition, we use the asymptotic notation from [9].

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 18; pp. 18:1–18:16
Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

▶ **Theorem 1** ([1, 14]). *Let $m = n/2 + s$, where $s = s(n) = o(n)$ and let $G = G(n, m)$. Then for every $i \in \mathbb{N}$ the following holds with high probability*[1]*.*

(i) *If $\frac{s^3}{n^2} \to -\infty$, then H_i is a tree and $|H_i| = (1/2 + o(1)) \frac{n^2}{s^2} \log \frac{|s|^3}{n^2}$.*

(ii) *If $\frac{s^3}{n^2} \to c \in \mathbb{R}$, then $|H_i| = \Theta_p\left(n^{2/3}\right)$.*

(iii) *If $\frac{s^3}{n^2} \to \infty$, then $|H_1| = (4 + o(1))\, s$. For $i \geq 2$, we have $|H_i| = o\left(n^{2/3}\right)$.*

This drastic change of the component structure at $m = n/2 + O\left(n^{2/3}\right)$ is called the *emergence of the giant component*. These results raised the question whether there are also phase transitions in other classes of random graphs. Łuczak and Pittel [15] considered this question for $F(n, m)$, a graph chosen uniformly at random from all vertex-labelled forests with n vertices and m edges. They showed that, analogous to $G(n, m)$, the giant component in $F(n, m)$ emerges at $m = n/2 + O\left(n^{2/3}\right)$. Kang and Łuczak [12] showed that the same is true for $P(n, m)$, a graph chosen uniformly at random from all vertex-labelled planar graphs with n vertices and $m = m(n)$ edges. Later Kang, Moßhammer, and Sprüssel [13] extended this result even to graphs on orientable surfaces.

Surprisingly, this problem for a random *outerplanar* graph is still open, although the class of outerplanar graphs lies "between" the class of forests and the class of planar graphs and therefore we expect similar behaviours. (A graph is outerplanar if it has an embedding in the plane in such a way that every vertex lies on the outer face, equivalently, a graph is outerplanar iff it contains neither K_4 nor $K_{2,3}$ as a minor.) In this paper we solve this open problem on the emergence of the giant component in a random outerplanar graph.

Kang, Moßhammer, and Sprüssel [13] used the core-kernel approach to obtain their results on the giant component in $S_g(n, m)$, a graph chosen uniformly at random from all vertex-labelled graphs with n vertices, $m = m(n)$ edges and genus at most g (for any constant $g \geq 0$). This method is mainly based on the following decomposition. We call a component of a graph G *complex* if it has at least two cycles. We decompose G into the *complex part* Q_G, which is the union of all complex components, and into non-complex components. Then we extract the *core* C_G, which is the maximal subgraph of Q_G of minimum degree at least two. Finally, we consider the *kernel* K_G, which can be obtained from C_G by the following operation. Every maximal path P consisting of vertices of degree two is replaced by an edge between the vertices of degree at least three that are adjacent to the end vertices of P. Conversely, starting from kernels (as base cases) we can construct cores by subdividing edges with additional vertices. Similarly, the complex part can be formed by replacing every vertex in the core by a rooted tree. Finally, we obtain the whole graph G by choosing the complex part and non-complex components.

However, we *cannot* apply the core-kernel approach to *outerplanar* graphs, because this method is mainly based on the fact that a graph G is embeddable on a surface if and only if its kernel K_G is. But an analogous statement for outerplanar graphs is not true, since a subdivision of an outerplanar graph is not necessarily outerplanar. Therefore, in this paper we shall start directly from cores (as base cases), not from the kernels. One of key steps in this direct core approach is to investigate how the number of outerplanar cores (and complex parts, respectively) changes by addition of a vertex and an edge. Using our core approach we prove that the giant component in a random outerplanar graph with n vertices and $m = m(n)$ edges emerges at $m = n/2 + O\left(n^{2/3}\right)$.

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[1] With probability tending to 1 as n tends to infinity, whp for short.

1.2 Main results

To state our main results we need to introduce some notations. Given a graph G, we define the excess of a complex component of G to be the difference between the number of its edges and the number of its vertices. The excess of G, denoted by $ex(G)$ or $\ell(G)$, is the sum of the excesses of all complex components of G. In addition, we denote by $n_C(G)$ the number of vertices in the core C_G. Let $A(n,m)$ denote a graph chosen uniformly at random from all vertex-labelled outerplanar graphs with n vertices and $m = m(n)$ edges.

▶ **Theorem 2.** *Let $m = n/2 + s$, where $s = s(n) = o(n)$ and let $G = A(n,m)$. For every $i \in \mathbb{N}$ whp the following holds.*

(i) *If $\frac{s^3}{n^2} \to -\infty$, then H_i is a tree and $|H_i| = (1/2 + o(1))\, \frac{n^2}{s^2} \log \frac{|s|^3}{n^2}$.*

(ii) *If $\frac{s^3}{n^2} \to c \in \mathbb{R}$, then $|H_i| = \Theta_p\left(n^{2/3}\right)$.*

(iii) *If $\frac{s^3}{n^2} \to \infty$, then $|H_1| = 2s + O_p\left(n^{2/3}\right)$. For $i \geq 2$, we have $|H_i| = \Theta_p\left(n^{2/3}\right)$. In addition, we have $n_C(G) = \Theta\left(sn^{-1/3}\right)$ and $ex(G) = \Theta\left(sn^{-2/3}\right)$.*

To prove Theorem 2 we shall use some auxiliary results about *cactus* graphs, which form a subfamily of the class of outerplanar graphs and are interesting in their own – a cactus graph is a graph in which every edge belongs to at most one cycle. A simple, but important observation is that a graph is a cactus graph if and only if its kernel is a cactus graph. Therefore, analogously to the case of random graphs on surfaces [13] we can apply the aforementioned core-kernel approach to obtain results on the component structure of a random cactus graph, such as the order of the largest component, the core, and the kernel. In addition, we determine the asymptotic number of cubic (i.e. 3-regular) cactus multigraphs using singularity analysis of generating functions which arise from the standard decomposition of graphs into smaller building blocks.

We denote by $T(n,m)$ a graph chosen uniformly at random from all vertex-labelled cactus graphs with n vertices and $m = m(n)$ edges. In addition, let $\mathcal{K}(2n,3n)$ be the class of all cubic cactus *weighted multigraphs* with $2n$ vertices and $3n$ edges, and $\mathcal{K}_c(2n,3n)$ be the subclass of $\mathcal{K}(2n,3n)$ containing all connected graphs. Here every multigraph K is counted with a weight of $w(K) = 2^{-e_1(K)-e_2(K)}$, where $e_1(K)$ denotes the number of loops in K and $e_2(K)$ the number of double edges (see [10, p.5] for details of the weight of a multigraph).

▶ **Theorem 3.**

(i) *Let $m = n/2 + s$, where $s = s(n)$, $n^{2/3} \ll s \ll n$ and $G = T(n,m)$. Then whp $|H_1| = 2s + O_p\left(n^{2/3}\right)$, $n_C(G) = \Theta\left(sn^{-1/3}\right)$, $ex(G) = \Theta\left(sn^{-2/3}\right)$, and the kernel K_G is cubic.*

(ii) *There are constants $c_0, c_1, \gamma > 0$ such that as $n \to \infty$,*

$$|\mathcal{K}(2n,3n)| = (1+o(1))c_0 n^{-5/2}\gamma^{2n}(2n)!,$$

$$\text{and} \qquad |\mathcal{K}_c(2n,3n)| = (1+o(1))c_1 n^{-5/2}\gamma^{2n}(2n)!.$$

Finally, we use Theorem 2 to show that when $m = n/2 + s$ for $n^{2/3} \ll s \ll n$, the two random graphs $A(n,m)$ and $T(n,m)$ are "contiguous", meaning that they are indistinguishable in view of properties that hold whp. Such a contiguity of two models will turn out to be very helpful for further investigations of the behaviour of $A(n,m)$, partly because the core-kernel approach is applicable for $T(n,m)$.

▶ **Theorem 4.** *Let $m = n/2 + s$, where $s = s(n)$ and $n^{2/3} \ll s \ll n$. Then, whp every edge in $A(n,m)$ belongs to at most one cycle. In other words, whp $A(n,m)$ is a cactus graph.*

2 Proof strategy of Theorem 2

We start with the cases $s^3/n^2 \to -\infty$ and $s^3/n^2 \to c \in \mathbb{R}$. By a well-known fact (see Lemma 12(i),(ii)) we obtain $\liminf_{n\to\infty} \mathbb{P}[G(n,m) \text{ is outerplanar}] > 0$. Thus, each property that holds whp in $G(n,m)$ is also true whp in $A(n,m)$ and the Statements (i) and (ii) follow from Theorem 1. Thus, it suffices to prove (iii), for which we use the direct core approach. To illustrate this approach, we introduce further notations.

▶ **Definition 5.** *We denote by*
- $\mathcal{A}$ *the class of all outerplanar graphs;*
- $\mathcal{Q}$ *the class of all complex outerplanar graphs (i.e. complex parts of graphs in* $\mathcal{A}$*);*
- $\mathcal{C}$ *the class of all complex outerplanar graphs with minimum degree at least two (i.e. cores of graphs in* $\mathcal{A}$*);*
- $\mathcal{U}$ *the class of all graphs without complex components.*

In addition, for any graph class $\mathcal{X}$ *we denote by* $\mathcal{X}(n,m)$ *the subclass containing those graphs with* n *vertices and* m *edges.*

▶ **Definition 6.** *Let* G *be a graph with* n *vertices and* m *edges. We denote by*
- $n_Q = n_Q(G)$ *the number of vertices in the complex part* Q_G*;*
- $n_C = n_C(G)$ *the number of vertices in the core* C_G*;*
- $\ell = \ell(G)$ *the excess of* G*, i.e. the difference between the number of edges and the number of vertices in the complex part* Q_G*;*
- $n_U = n_U(G) := n - n_Q$ *the number of vertices in* G *outside the complex part* Q_G*;*
- $m_U = m_U(G) := m - n_Q - \ell$ *the number of edges in* G *outside the complex part* Q_G *(with* n_Q *vertices and* $n_Q + \ell$ *edges).*

We reverse the decomposition in the core approach to obtain relations between the classes defined above. We observe that each outerplanar graph can be constructed in a unique way by combining a complex graph and non-complex components. Similarly, a complex graph can be formed by choosing the core and replacing each vertex of the core by a rooted tree. It is well known that we have $n_C n_Q^{n_Q-n_C-1}$ different possibilities for choosing these trees (see e.g. [17]). Hence, we obtain

$$|\mathcal{A}(n,m)| = \sum\nolimits_{n_Q,\ell} \binom{n}{n_Q} |\mathcal{Q}(n_Q, n_Q+\ell)| \cdot |\mathcal{U}(n_U, m_U)| = \sum\nolimits_{n_Q,\ell} \tau(n_Q,\ell), \tag{1}$$

$$|\mathcal{Q}(n_Q, n_Q+\ell)| = \sum\nolimits_{n_C} \binom{n_Q}{n_C} |\mathcal{C}(n_C, n_C+\ell)| n_C n_Q^{n_Q-n_C-1} = \sum\nolimits_{n_C} \rho(n_C), \tag{2}$$

where we define

$$\tau(n_Q,\ell) := \binom{n}{n_Q} |\mathcal{Q}(n_Q, n_Q+\ell)| \cdot |\mathcal{U}(n_U, m_U)|,$$
$$\rho(n_C) := \binom{n_Q}{n_C} |\mathcal{C}(n_C, n_C+\ell)| n_C n_Q^{n_Q-n_C-1}.$$

In the sums of (1) and (2) we did not specify precisely in which sets the summation indices lie. But it is convenient to consider only terms, which are non-zero. We call the corresponding indices *admissible*. The next step is to find in the sums (1) and (2) those terms, which are significantly larger than the other ones. In order to make that more precise, we use the following terminology.

▶ **Definition 7.** *For each $n \in \mathbb{N}$ let $I_0(n), I(n) \subseteq \mathbb{N}$ be finite index sets such that $I_0(n) \subseteq I(n)$. In addition, let $\sigma_n(i) \geq 0$ for each $i \in I(n)$. Then the main contribution to the sum $\sum_{i \in I(n)} \sigma_n(i)$ is provided by $i \in I_0(n)$ if $\sum_{i \in I(n) \setminus I_0(n)} \sigma_n(i) = o\left(\sum_{i \in I(n)} \sigma_n(i)\right)$ for $n \to \infty$. In that case, we also say that the terms provided by $i \in I(n) \setminus I_0(n)$ are negligible.*

Now the goal is to find sets I_{n_Q}, I_ℓ and I_{n_C} such that the main contributions to (1) and (2) are provided by $n_Q \in I_{n_Q}, \ell \in I_\ell$, and $n_C \in I_{n_C}$. Having such sets we immediately get results about the structure of a random outerplanar graph $G = A(n, m)$. Namely, that whp $n_Q(G) \in I_{n_Q}, \ell(G) \in I_\ell$, and $n_C(G) \in I_{n_C}$. To get strong results, we aim to find sets I_{n_Q}, I_ℓ, and I_{n_C}, which are as small as possible. Afterwards we use this concentration information and a double counting argument (see Lemma 21) to deduce the component structure of G. The main challenge is to determine I_{n_Q}, I_ℓ, and I_{n_C}.

In order to illustrate our main idea of the analysis of the sums (1) and (2), we consider the generic sums $\Sigma_n = \sum_{i \in I(n)} \sigma_n(i)$ from Definition 7. The goal is to find "small" sets $I_0(n)$ such that the main contribution to Σ_n is provided by $i \in I_0(n)$ or equivalently "large" sets $I_1(n)$ such that the terms provided by $i \in I_1(n)$ are negligible in Σ_n. Our method to find these sets $I_1(n)$ is mainly based on the following observation.

▶ **Lemma 8.** *For each $n \in \mathbb{N}$ let $I_1(n), I(n) \subseteq \mathbb{N}$ be finite index sets such that $I_1(n) \subseteq I(n)$ and let $\sigma_n(i) \geq 0$ for each $i \in I(n)$. In addition, for each $n \in \mathbb{N}$ let $f_n : I_1(n) \to I(n)$ be a function. We assume that there are a function ε with $\varepsilon(n) = o(1)$ and a constant $M > 0$ such that for all $n \in \mathbb{N}, i \in I_1(n)$ and $j \in I(n)$*

$$\frac{\sigma_n(i)}{\sigma_n\left(f_n(i)\right)} \leq \varepsilon(n), \tag{3}$$

$$\textit{and} \qquad \left|f_n^{-1}\left(\{j\}\right)\right| \leq M. \tag{4}$$

Then the terms provided by $i \in I_1(n)$ are negligible in $\sum_{i \in I(n)} \sigma_n(i)$.

In most cases when we apply Lemma 8, the functions f_n will be of the form $f_n(i) = i + g(n)$ for some function $g : \mathbb{N} \to \mathbb{Z}$ or of the form $f_n(i) = \lfloor \delta i \rfloor$ for some constant $\delta > 0$. We note that such functions f_n always fulfil (4) for some $M > 0$. Thus, it remains to find a function ε with $\varepsilon(n) = o(1)$ such that (3) is satisfied. For simplicity, we demonstrate our method of doing that only for the case when $f_n(i) = i + g(n)$ for some function g with $g(n) > 0$. Moreover, we assume that $I(n) = \{a_n, a_n + 1, \ldots, b_n\}$ for some $a_n < b_n$. We observe that

$$\frac{\sigma_n(i)}{\sigma_n(f_n(i))} = \frac{\sigma_n(i)}{\sigma_n(i + g(n))} = \prod_{k=i}^{i+g(n)-1} \frac{\sigma_n(k)}{\sigma_n(k+1)}. \tag{5}$$

Thus, we aim to find good upper bounds for $\frac{\sigma_n(k)}{\sigma_n(k+1)}$. We commonly state these bounds in the form $\exp(h(n))$ for some function $h : \mathbb{N} \to \mathbb{R}$. Then, if we assume

$$\frac{\sigma_n(k)}{\sigma_n(k+1)} \leq \exp(h(n)), \qquad \forall n \in \mathbb{N}, \forall k \in \{i, \ldots, i + g(n) - 1\}, \tag{6}$$

we get together with (5), $\frac{\sigma_n(i)}{\sigma_n(f_n(i))} \leq \exp\left(g(n)h(n)\right)$. If we find such functions g and h with $g(n)h(n) \to -\infty$ for $n \to \infty$, then we can apply Lemma 8 (see Appendix A for an application of Lemma 8). We can summarise the above idea as follows. The key for a good analysis of the sum $\sum_{i \in I(n)} \sigma_n(i)$ is to have good bounds for the fractions $\frac{\sigma_n(k)}{\sigma_n(k+1)}$ or equivalently good bounds for $\frac{\sigma_n(k+1)}{\sigma_n(k)}$.

Now we describe how we find these bounds for the sums in (1) and (2). In order to find good bounds for $\frac{\rho(n_C+1)}{\rho(n_C)}$, it suffices to estimate $\frac{|\mathcal{C}(n_C+1,n_C+1+\ell)|}{|\mathcal{C}(n_C,n_C+\ell)|}$ (see Lemma 9). To that end, we construct graphs in $\mathcal{C}\left(n_C+1, n_C+1+\ell\right)$ as follows: Let $H \in \mathcal{C}(n_C, n_C+\ell)$ and an edge e of H be given. Then we obtain in "most" cases a graph $H' \in \mathcal{C}(n_C+1, n_C+1+\ell)$ if we subdivide e by one vertex and label this new vertex with n_C+1. By a careful analysis of this construction we will obtain good estimates for $\frac{\rho(n_C+1)}{\rho(n_C)}$.

In the next step we consider the sum in (1) and shall determine I_{n_Q} and I_ℓ. To that end, we look at the fractions $\frac{\tau(n_Q+1,\ell)}{\tau(n_Q,\ell)}$ and $\frac{\tau(n_Q,\lfloor\delta\ell\rfloor)}{\tau(n_Q,\ell)}$ for a constant $\delta > 0$. To get bounds for the term $|\mathcal{U}(n_U, m_U)|$, we will use Lemma 12. Thus, it remains to find estimates for $\frac{|\mathcal{Q}(n_Q+1,n_Q+1+\ell)|}{|\mathcal{Q}(n_Q,n_Q+\ell)|}$ and $\frac{|\mathcal{Q}(n_Q,n_Q+\lfloor\delta\ell\rfloor)|}{|\mathcal{Q}(n_Q,n_Q+\ell)|}$. For the first fraction (see Lemma 13) we define for $i \in \{0, 1\}$

$$\rho_i(n_C) = \rho_i(n_C, n_Q, \ell) := \binom{n_Q+i}{n_C} |\mathcal{C}(n_C, n_C+\ell)|\, n_C (n_Q+i)^{n_Q+i-n_C-1}.$$

With this notation we have

$$\frac{|\mathcal{Q}(n_Q+1, n_Q+1+\ell)|}{|\mathcal{Q}(n_Q, n_Q+\ell)|} = \frac{\sum_{n_C} \rho_1(n_C)}{\sum_{n_C} \rho_0(n_C)}. \tag{7}$$

From the analysis of (2) we already know sets I_0, I_1 such that the main contributions to $\sum_{n_C} \rho_0(n_C)$ and $\sum_{n_C} \rho_1(n_C)$ are provided by $n_C \in I_0$ and $n_C \in I_1$, respectively. We will see that we may assume $I := I_0 = I_1$. Then we will get a good bound for (7) if for $n_C \in I$ we estimate the fraction

$$\frac{\rho_1(n_C)}{\rho_0(n_C)} = \frac{(n_Q+1)^2}{n_Q-n_C+1} \left(\frac{n_Q+1}{n_Q}\right)^{n_Q-n_C-1}. \tag{8}$$

For the fraction $\frac{|\mathcal{Q}(n_Q,n_Q+\lfloor\delta\ell\rfloor)|}{|\mathcal{Q}(n_Q,n_Q+\ell)|}$ (see Lemma 16), we will use that

$$\frac{|\mathcal{Q}_C(n_Q, n_Q+\lfloor\delta\ell\rfloor)|}{|\mathcal{Q}_P(n_Q, n_Q+\ell)|} \leq \frac{|\mathcal{Q}(n_Q, n_Q+\lfloor\delta\ell\rfloor)|}{|\mathcal{Q}(n_Q, n_Q+\ell)|} \leq \frac{|\mathcal{Q}_P(n_Q, n_Q+\lfloor\delta\ell\rfloor)|}{|\mathcal{Q}_C(n_Q, n_Q+\ell)|}, \tag{9}$$

where $\mathcal{Q}_P(n_Q, n_Q+\ell)$ denotes the class of all complex planar graphs with n_Q vertices and $n_Q+\ell$ edges and $\mathcal{Q}_C(n_Q, n_Q+\ell)$ the class of all complex cactus graphs with n_Q vertices and $n_Q+\ell$ edges. We get estimates for $|\mathcal{Q}_C(n_Q, n_Q+\ell)|$ and $|\mathcal{Q}_P(n_Q, n_Q+\ell)|$ by using the core-kernel approach (see Lemmas 14 and 15). In order to show that these bounds are tight enough, we make the following observations. We will see that there is a constant $c > 0$ such that

$$\frac{|\mathcal{Q}_P(n_Q, n_Q+\ell)|}{|\mathcal{Q}_C(n_Q, n_Q+\ell)|} \leq c^\ell, \tag{10}$$

Thus, we make a multiplicative error of at most c^ℓ if we use $|\mathcal{Q}_P(n_Q, n_Q+\ell)|$ as an estimate for $|\mathcal{Q}(n_Q, n_Q+\ell)|$. We observe that the possible error increases at most by the constant factor c if we increase ℓ by one. On the other hand, we will get $\frac{\tau(n_Q,\ell+1)}{\tau(n_Q,\ell)} \approx \Theta(1)\frac{n_Q^{3/2}}{\ell^{3/2}}\frac{1}{n}$. Hence, $\tau(n_Q, \ell)$ decays in ℓ outside the range $\ell = \Theta\left(n_Q n^{-2/3}\right)$ "much faster" than the growth of the error in (10). Having found estimates for $\frac{|\mathcal{Q}(n_Q+1,n_Q+1+\ell)|}{|\mathcal{Q}(n_Q,n_Q+\ell)|}$ and $\frac{|\mathcal{Q}(n_Q,n_Q+\lfloor\delta\ell\rfloor)|}{|\mathcal{Q}(n_Q,n_Q+\ell)|}$, we obtain bounds for $\frac{\tau(n_Q+1,\ell)}{\tau(n_Q,\ell)}$ and $\frac{\tau(n_Q,\lfloor\delta\ell\rfloor)}{\tau(n_Q,\ell)}$. Then we can apply Lemma 8 to find I_{n_Q} and I_ℓ.

3 Cores and complex parts: proof of Theorem 2

We recall that for a given graph G we denote by n_C the number of vertices in the core C_G and by ℓ the excess of G. In addition, $\mathcal{C}$ is the class of all outerplanar cores. Now we use the ideas presented in Section 2 and start by finding I_{n_C}. To that end, we obtain the following estimates for $\frac{|\mathcal{C}(n_C+1,n_C+1+\ell)|}{|\mathcal{C}(n_C,n_C+\ell)|}$.

▶ **Lemma 9.**
(i) *For all admissible n_C and ℓ we have*

$$\frac{|\mathcal{C}(n_C+1,n_C+1+\ell)|}{|\mathcal{C}(n_C,n_C+\ell)|} \geq n_C + \frac{\ell}{80}.$$

(ii) *If in addition $n_C - 8\ell \geq 0$, then*

$$\frac{|\mathcal{C}(n_C+1,n_C+1+\ell)|}{|\mathcal{C}(n_C,n_C+\ell)|} \leq (n_C+\ell)\frac{n_C+1}{n_C+1-8\ell}.$$

Using Lemma 9 we obtain bounds for $\frac{\rho(n_C+1)}{\rho(n_C)}$, which we can use to analyse the sum in (2) and find I_{n_C}. The following two lemmas state that we can choose $I_{n_C} = \Theta\left(\sqrt{n_Q\ell}\right)$, provided that $\ell = \omega(1)$. In Lemmas 18 and 19 we shall see that we may assume $\ell = \omega(1)$.

▶ **Lemma 10.** *There are $b, c > 0$ such that for all admissible n_Q and ℓ, we have*

$$\sum\nolimits_{n_C \leq c\sqrt{n_Q\ell}} \rho(n_C) \leq \exp(-b\ell) \sum\nolimits_{n_C} \rho(n_C).$$

▶ **Lemma 11.** *For all admissible n_Q, ℓ and $c \geq 14$, we have*

$$\sum\nolimits_{n_C \geq c\sqrt{n_Q\ell}} \rho(n_C) \leq \exp\left(-\frac{c}{2}\ell\right) \sum\nolimits_{n_C} \rho(n_C).$$

Next, we recall that $\mathcal{U}$ is the class of all graphs without complex components and $\mathcal{Q}$ the class of all complex outerplanar graphs. In addition, for a given graph G we denote by n_Q the number of vertices in the complex part Q_G, by n_U the number of vertices outside the complex part and by m_U the number of edges outside the complex part. We aim to find I_{n_Q} and I_ℓ by analysing $\frac{\tau(n_Q+1,\ell)}{\tau(n_Q,\ell)}$ and $\frac{\tau(n_Q,\lfloor\delta\ell\rfloor)}{\tau(n_Q,\ell)}$. To that end, we need the following estimates for $|\mathcal{U}(n_U, m_U)|$.

▶ **Lemma 12** ([3, 10, 13])**.** *Let $m = n/2 + s$ with $s = s(n) < n/2$ and $u(n,m) := |\mathcal{U}(n,m)|\binom{\binom{n}{2}}{m}^{-1}$. Then there is a constant $c > 0$ such that for*

$$f(n,m) := c\left(\frac{2}{e}\right)^{2m-n} \frac{m^{m+1/2}n^{n-2m+1/2}}{(n-m)^{n-m+1/2}},$$

we have
(i) *$u(n,m) \to 1$, if $\frac{s^3}{n^2} \to -\infty$;*
(ii) *for each $a \in \mathbb{R}$, there exists a constant $b > 0$ such that $u(n,m) \geq b$, whenever $s \leq an^{2/3}$;*
(iii) *$u(n,m) \leq n^{-1/2} f(n,m)$, if $0 < s \leq \frac{n^{3/4}}{2}$;*
(iv) *$u(n,m) \leq f(n,m)$, if $s > 0$.*

In addition, we use Lemmas 10 and 11 and (8) to obtain estimates for $\frac{|\mathcal{Q}(n_Q+1,n_Q+1+\ell)|}{|\mathcal{Q}(n_Q,n_Q+\ell)|}$.

▶ **Lemma 13.** *There exist constants $a_1, a_2, \varepsilon > 0$ and $K \in \mathbb{N}$ such that for all admissible n_Q and ℓ with $K \le \ell \le \varepsilon n_Q$, we have*

$$(n_Q+1)\exp\left(1+a_1\frac{\ell}{n_Q}\right) \le \frac{|\mathcal{Q}(n_Q+1, n_Q+1+\ell)|}{|\mathcal{Q}(n_Q, n_Q+\ell)|} \le (n_Q+1)\exp\left(1+a_2\frac{\ell}{n_Q}\right).$$

Next, we estimate $\frac{|\mathcal{Q}(n_Q, n_Q+\lfloor\delta\ell\rfloor)|}{|\mathcal{Q}(n_Q, n_Q+\ell)|}$ by using (9). To that end, we need the following two results, which can be obtained by using the core-kernel approach.

▶ **Lemma 14.** *There exist constants $a_1, a_2, \gamma, K, \varepsilon > 0$ and $b_1, b_2 \in \mathbb{R}$ such that for all admissible n_Q and ℓ with $K \le \ell \le \varepsilon n_Q$, we have*

$$|\mathcal{Q}_C(n_Q, n_Q+\ell)| \ge a_1 n_Q^{n_Q+3\ell/2-1/2}\gamma^\ell \ell^{-3\ell/2-2}\exp\left(b_1\sqrt{\ell^3 n_Q^{-1}}\right);$$
$$|\mathcal{Q}_C(n_Q, n_Q+\ell)| \le a_2 n_Q^{n_Q+3\ell/2-1/2}\gamma^\ell \ell^{-3\ell/2-2}\exp\left(b_2\sqrt{\ell^3 n_Q^{-1}}\right).$$

▶ **Lemma 15** ([13]). *There exist constants $a_3, a_4, \gamma_1, K, \varepsilon > 0$ and $b_3, b_4 \in \mathbb{R}$ such that for all admissible n_Q and ℓ with $K \le \ell \le \varepsilon n_Q$, we have*

$$|\mathcal{Q}_P(n_Q, n_Q+\ell)| \ge a_3 n_Q^{n_Q+3\ell/2-1/2}\gamma_1^\ell \ell^{-3\ell/2-3}\exp\left(b_3\sqrt{\ell^3 n_Q^{-1}}\right);$$
$$|\mathcal{Q}_P(n_Q, n_Q+\ell)| \le a_4 n_Q^{n_Q+3\ell/2-1/2}\gamma_1^\ell \ell^{-3\ell/2-3}\exp\left(b_4\sqrt{\ell^3 n_Q^{-1}}\right).$$

▶ **Lemma 16.** *There exist constants $c_1, c_2, K, \varepsilon > 0$ and $\delta \in (0,1)$ such that for all admissible n_Q and ℓ with $K \le \ell \le \varepsilon n_Q$, we have*

$$c_1^\ell\left(\frac{n_Q}{\ell}\right)^{3/2(\lfloor\delta\ell\rfloor-\ell)} \le \frac{|\mathcal{Q}(n_Q, n_Q+\lfloor\delta\ell\rfloor)|}{|\mathcal{Q}(n_Q, n_Q+\ell)|} \le c_2^\ell\left(\frac{n_Q}{\ell}\right)^{3/2(\lfloor\delta\ell\rfloor-\ell)}.$$

In order to apply Lemmas 13 and 16, we need the condition $K \le \ell \le \varepsilon n_Q$. The next lemma shows that this is indeed not a restriction for our considerations.

▶ **Lemma 17.** *Let $m = m(n) = n/2 + s$, where $s = s(n)$ and $n^{2/3} \ll s \ll n$. Then for each $K \in \mathbb{N}$ and $\varepsilon > 0$ the main contribution to $\sum_{n_Q,\ell}\tau(n_Q,\ell)$ is provided by n_Q and ℓ with $K \le \ell \le \varepsilon n_Q$.*

In Lemma 12 we observe that $u(n_U, m_U)$ stays close to one, as long as $n_U \ge 2m_U$. Thus, we will use in that case $\binom{\binom{n_U}{2}}{m_U}$ as an estimate for $|\mathcal{U}(n_U, m_U)|$. In contrast, $u(n_U, m_U)$ starts becoming quite small if $n_U < 2m_U$. Hence, in that case we will use stronger bounds given by Lemma 12(iii) and (iv). Thus, we define

$$T_1 := \sum\nolimits_{n_U \ge 2m_U}\tau(n_Q,\ell) \quad \text{and} \quad T_2 := \sum\nolimits_{n_U < 2m_U}\tau(n_Q,\ell).$$

▶ **Lemma 18.** *Let $m = m(n) = n/2 + s$, where $s = s(n)$ and $n^{2/3} \ll s \ll n$. Then the main contribution to $T_1 = \sum_{n_U \ge 2m_U}\tau(n_Q,\ell)$ is provided by $n_Q = 2s + O_p\left(n^{2/3}\right)$ and $\ell = \Theta\left(sn^{-2/3}\right)$.*

▶ **Lemma 19.** *Let $m = m(n) = n/2 + s$, where $s = s(n)$ and $n^{2/3} \ll s \ll n$. Then the main contribution to $T_2 = \sum_{n_U < 2m_U}\tau(n_Q,\ell)$ is provided by $n_Q = 2s + O_p\left(n^{2/3}\right)$ and $\ell = \Theta\left(sn^{-2/3}\right)$.*

Combining Lemmas 18 and 19 we can choose $I_{n_Q} = 2s + O_p\left(n^{2/3}\right)$ and $I_\ell = \Theta\left(sn^{-2/3}\right)$. Thus, we also obtain $I_{n_C} = \Theta\left(\sqrt{n_Q \ell}\right) = \Theta\left(sn^{-1/3}\right)$. This leads to the following results on the asymptotic order of the core and excess.

▶ **Lemma 20.** *Let $m = m(n) = n/2 + s$, where $s = s(n)$ and $n^{2/3} \ll s \ll n$, and let $G = A(n,m)$. Then whp $n_C(G) = \Theta\left(sn^{-1/3}\right)$ and $ex(G) = \Theta\left(sn^{-2/3}\right)$.*

In order to obtain the order of the largest component, we look at the complex part Q_G. Intuitively we expect that the largest component of Q_G is also the largest in G. The following lemma tells us that this is indeed the case.

▶ **Lemma 21.** *Let $m = m(n) = n/2 + s$, where $s = s(n)$ and $n^{2/3} \ll s \ll n$. Moreover, let $G = A(n,m)$. Then $n_Q(G) - |H_1(Q_G)| = O_p\left(n^{2/3}\right)$.*

Lemma 21 together with $I_{n_Q} = 2s + O_p\left(n^{2/3}\right)$ implies that the complex part Q_G has one component with $2s + O_p\left(n^{2/3}\right)$ vertices, while all other components are of order $O_p\left(n^{2/3}\right)$. For the non-complex components we observe that $m_U = n_U/2 + O_p\left(n_U^{2/3}\right)$. Thus, for each $i \in \mathbb{N}$ the $i-$th largest non-complex component has $\Theta_p\left(n^{2/3}\right)$ vertices by Theorem 1 and Lemma 12. This concludes the proof of Theorem 2.

4 Singularity analysis: proof of Theorem 3

It suffices to show Theorem 3(ii), since (i) follows from (ii) and Remark 8.6 in [13]. We denote by $\mathcal{K}_c^\circ$ the class of connected cubic cactus weighted multigraphs, where one vertex is marked. Moreover, let $\mathcal{B}$ be the class of connected cactus weighted multigraphs, where all but one vertex have degree three and the exceptional vertex has degree two. We denote by $B(z), K(z), K_c(z)$ and $K_c^\circ(z)$ the exponential generating functions of the classes $\mathcal{B}, \mathcal{K}, \mathcal{K}_c$, and $\mathcal{K}_c^\circ$, respectively. By considering the marked vertex of a graph in $\mathcal{K}_c^\circ$ and distinguish some cases we obtain

$$K_c^\circ(z) = \frac{zB(z)}{2(1 - zB(z))} + \frac{zB(z)^3}{6}.$$

Similarly, by considering the vertex of degree two in graphs in $\mathcal{B}$ we get

$$B(z) = \frac{z}{2(1 - zB(z))} + \frac{z}{2}B(z)^2. \tag{11}$$

We observe that the even coefficients in $B(z)$ are all zero, i.e. $B(z) = \sum_{i \geq 1} b_{2i-1} z^{2i-1}$ for some $b_{2i-1} \in \mathbb{N}$. By taking $\widetilde{B}(u) := \sum_{i \geq 1} b_{2i-1} u^i$, we observe that (11) translates to

$$\widetilde{B}(u) = \frac{u}{2\left(1 - \widetilde{B}(u)\right)} + \frac{1}{2}\widetilde{B}(u)^2.$$

Using techniques from [4, 7] we obtain that for $u \to r$,

$$\widetilde{B}(u) = t - \rho\sqrt{1 - \frac{u}{r}} + O\left(1 - \frac{u}{r}\right),$$

where $t = 1 - \frac{\sqrt{3}}{3}$, $r = \frac{2\sqrt{3}}{9}$, and $\rho = \frac{\sqrt{2}}{3}$. Moreover, r is the unique dominant singularity of $\widetilde{B}(u)$, due to the aperiodicity of $\widetilde{B}(u)$. Next, we define $\widetilde{K}_c^\circ(u) := K_c^\circ(\sqrt{u})$, $\widetilde{K}_c(u) := K_c(\sqrt{u})$ and $\widetilde{K}(u) := K(\sqrt{u})$. Using $u \cdot \widetilde{K}_c^\circ(u) = \widetilde{B}(u)^2 - \widetilde{B}(u)^3/3$ and $K_c(z) = \int K_c^\circ(z)/z \mathrm{d}z$ we obtain that there are $k_1, k_2, k_3 \in \mathbb{R}$ such that for $u \to r$

$$\widetilde{K}_c(u) = k_1 + k_2\left(1 - \frac{u}{r}\right) + k_3\left(1 - \frac{u}{r}\right)^{\frac{3}{2}} + O\left(\left(1 - \frac{u}{r}\right)^2\right).$$

Hence, there is a constant $c_1 > 0$ such that with $\gamma := r^{-1/2}$ we obtain

$$\left[z^{2n}\right] K_c(z) = [u^n]\,\widetilde{K}_c(u) = c_1 \gamma^{2n} n^{-\frac{5}{2}}\left(1 + o(1)\right), \quad \text{as} \quad n \to \infty.$$

Finally, we use $\widetilde{K}(u) = \exp\left(\widetilde{K}_c(u)\right)$ to obtain that there is a $c_0 > 0$ such that $\left[z^{2n}\right] K(z) = [u^n]\,\widetilde{K}(u) = c_0 \gamma^{2n} n^{-\frac{5}{2}}\left(1 + o(1)\right)$ for $n \to \infty$.

5 Blocks and chords: proof of Theorem 4

We will use a double counting argument to show Theorem 4. To that end, we need some structural information about $G = A(n, m)$. By Lemma 20 we know that whp $n_C(G) = \Theta\left(sn^{-1/3}\right)$ and $ex(G) = \ell(G) = \Theta\left(sn^{-2/3}\right)$. Apart from that we need the two following lemmas about blocks and chords, where we call a maximal 2-connected subgraph of G a *block*. In addition, a *chord* is an edge in G that lies in a block B, but not in the unique Hamiltonian cycle of B.

▶ **Lemma 22.** *Let $m = m(n) = n/2 + s$, where $s = s(n)$ and $n^{2/3} \ll s \ll n$. Then whp $A(n, m)$ does not contain a vertex that lies in three blocks.*

Given a chord xy, we denote by B_{xy} the block that contains x and y and by B'_{xy} the unique Hamiltonian cycle of B_{xy}. A chord xy is said to be *good* (with respect to a function $h(n) = \omega(1)$) if there is a path $P_{xy} = z_0 z_1 \dots z_r z_{r+1}$ from $z_0 = x$ to $z_{r+1} = y$ in B'_{xy} such that

- $z_1, \dots, z_r$ are not endpoints of any chords in B_{xy};
- $r \geq n^{1/3} h(n)^{-1} + 1$;
- z_i has degree 2 for all $i \in \mathbb{N}$ with $1 \leq i \leq n^{1/3} h(n)^{-1}$.

▶ **Lemma 23.** *Let $m = m(n) = n/2 + s$, where $s = s(n)$ and $n^{2/3} \ll s \ll n$ and $h(n) = \omega(1)$. Then whp $A(n, m)$ has either no chord or a good chord xy (with respect to $h(n)$).*

Now we fix $h(n) = \omega(1)$ such that $sh(n) = o(n)$. We denote by $\mathcal{A}'(n, m)$ the subclass of $\mathcal{A}(n, m)$ containing those graphs H that have a good chord, have no vertex lying in three blocks, and satisfies $n_C(H) = \Theta\left(sn^{-1/3}\right)$ and $\ell(H) = \Theta\left(sn^{-2/3}\right)$. Due to Theorem 2 and Lemmas 22 and 23, it suffices to show $|\mathcal{A}'(n, m)| = o\left(|\mathcal{A}(n, m)|\right)$. To that end, we consider the following operation for $H \in \mathcal{A}'(n, m)$:

- We choose a good chord xy and denote by $P_{xy} = z_0 z_1 \dots z_r z_{r+1}$ the corresponding good path from $z_0 = x$ to $z_{r+1} = y$.
- We choose $i \in \mathbb{N}$ with $1 \leq i \leq n^{1/3} h(n)^{-1}$.
- We add the edge $z_i z_r$ and delete $z_r y$.

We observe that we have at least $n^{1/3} h(n)^{-1} - 1$ options for performing this operation. In addition, we note that the following holds in the new graph H' resulting from H by the above operation:

- $H' \in \mathcal{A}(n, m)$, $n_C(H') = n_C(H)$, and $\ell(H') = \ell(H)$;
- z_i has degree 3;
- z_i and z_r are neighbours;
- there is a path from z_i to x such that all internal vertices have degree two;
- x lies in at most two blocks;
- y is a neighbour of x such that xy lies in the unique Hamiltonian cycle of the block containing x and y.

Thus, for a fixed graph H' there are at most $2\ell \cdot 3 \cdot 3 \cdot 4 = \Theta\left(sn^{-2/3}\right)$ many different graphs H such that we can obtain H' by performing our operation in H. Hence, we obtain $|\mathcal{A}'(n, m)| = O\left(\frac{sn^{-2/3}}{n^{1/3} h(n)^{-1}}\right) |\mathcal{A}(n, m)| = o\left(|\mathcal{A}(n, m)|\right)$.

6 Sketches of proofs of auxiliary results

Proof of Lemma 9. For a graph $H \in \mathcal{C}(n_C, n_C+\ell)$ we consider the following two constructions for building a graph in $\mathcal{C}(n_C+1, n_C+1+\ell)$:

(C1) We choose an edge e of H which is not a chord. Then we subdivide e by one vertex and label this new vertex with n_C+1.

(C2) We choose a vertex v in H of degree 3, 4, 5 or 6 and an edge e which is incident to v and not a chord. Then we relabel v with label n_C+1 and subdivide e by one vertex which obtain the label of v.

We observe that if H has b chords, then we have $n_C+\ell-b$ options for performing (C1). In addition, H has at least $b/2$ vertices of degree at least three and at most $2\ell/5$ vertices of degree at least seven. Hence, we have at least $b/2-2\ell/5$ choices for performing (C2). Now if $b \leq 19\ell/20$, then we have at least $n_C+\ell/20$ choices for (C1). Otherwise if $b > 19\ell/20$, then we have at least n_C choices for (C1) and at least $3\ell/40$ options for (C2). We note that each graph $H' \in \mathcal{C}(n_C+1, n_C+1+\ell)$ can be obtained at most once by performing (C1) and if this is the case, then it cannot be obtained by (C2). Finally, observing that H' can be obtained at most six times by performing (C2) yields statement (i).

For (ii) we call a vertex v of $H' \in \mathcal{C}(n_C+1, n_C+1+\ell)$ *nice* if it has degree two and the two neighbours are not adjacent. We observe that H' can be obtained by (C1) if the vertex n_C+1 is nice. We note that if v has degree two and is not nice, then v has a neighbour of degree at least three. Thus, H' has at least $n_C+1-8\ell$ nice vertices, since the sum of all degrees of vertices of degree at least three is at most 6ℓ. As H' was arbitrary, (ii) follows. ◀

The statements of Lemmas 10, 11 and 17-19 are all of the type that they determine the main contribution to some sum. In order to show these results we use Lemma 8, which usually requires a long and technical computation. Therefore, we provide only sketches of these proofs in this chapter, but we shall give a full proof of Lemma 10 in Appendix A to illustrate how to work out the details.

Proof of Lemma 10 and 11. If ℓ is "small" compared to n_C, we get by Lemma 9 that $\frac{|\mathcal{C}(n_C+1,n_C+1+\ell)|}{|\mathcal{C}(n_C,n_C+\ell)|} = n_C + \Theta(1)\ell$. Using this, we obtain $\frac{\rho(n_C+1)}{\rho(n_C)} = \left(1-\frac{n_C}{n_Q}\right)\left(1+\Theta(1)\frac{\ell}{n_C}\right)$. Hence, we expect that the main contribution to (2) is provided by terms with $n_C = \Theta\left(\sqrt{n_Q\ell}\right)$. ◀

Proof of Lemma 13. Combining Lemmas 10 and 11 together with (8) we obtain

$$\frac{|\mathcal{Q}(n_Q+1, n_Q+1+\ell)|}{|\mathcal{Q}(n_Q, n_Q+\ell)|} \approx \frac{\rho_1\left(\sqrt{n_Q\ell}\right)}{\rho_0\left(\sqrt{n_Q\ell}\right)}$$
$$\approx (n_Q+1)\exp\left(\frac{\sqrt{n_Q\ell}}{n_Q-\sqrt{n_Q\ell}+1} + \frac{n_Q-\sqrt{n_Q\ell}-1}{n_Q}\right) \approx (n_Q+1)\exp\left(1+\frac{\ell}{n_Q}\right). \quad ◀$$

Proof of Lemma 14. Using the core-kernel approach from [13] and following the lines of the proofs of Lemma 4.9(ii) and Corollary 4.11 in [13] yields the assertion. (A detailed proof can be found in Appendix B). ◀

Proof of Lemma 16. We note that $\ell = O(n_Q)$, which implies $\exp\left(\Theta(1)\sqrt{\ell^3 n_Q^{-1}}\right) = \exp\left(\Theta(1)\,\ell\right)$. Then the statement follows by combining Lemmas 14 and 15 together with (9). ◀

Proof of Lemma 17. We denote by $\mathcal{T}$ the class of cactus graphs. Clearly, we have $|\mathcal{A}(n,m)| \geq |\mathcal{T}(n,m)|$, because every cactus graph is also an outerplanar graph. By the core-kernel approach we obtain that there is a $c>0$ and $N \in \mathbb{N}$ such that $|\mathcal{T}(n,m)| \geq \frac{n^{n-1/2}}{(n-2s)^{n/2-s}} \exp\left(\frac{n}{2}-s+c\cdot\frac{s}{n^{2/3}}\right)$ for all $n \geq N$. On the other hand, we can bound $\tau(n_Q,\ell)$ by Lemmas 12 and 15. By doing so we obtain that $\sum_{\ell<K,n_Q}\tau(n_Q,\ell) = o\left(|\mathcal{T}(n,m)|\right)$. Hence, the terms provided by $\ell<K$ are negligible in $\sum_{n_Q,\ell}\tau(n_Q,\ell)$. Similarly, one can also show that this is true for the terms provided by $\ell > \varepsilon n_Q$. ◀

Proof of Lemma 18. By Lemma 12 we may consider $Y_1 = \sum_{n_U \geq 2m_U} \upsilon_1(n_Q,\ell)$ instead of T_1, where $\upsilon_1(n_Q,\ell) := \binom{n}{n_Q}|\mathcal{Q}(n_Q,n_Q+\ell)|\binom{\binom{n_U}{2}}{m_U}$. Then we obtain by Lemma 16 that $\frac{\upsilon_1(n_Q,\lfloor\delta\ell\rfloor)}{\upsilon_1(n_Q,\ell)} = \left(\Theta(1)\frac{n_Q^{3/2}m_U}{\ell^{3/2}n^2}\right)^{\lfloor\delta\ell\rfloor-\ell}$. Thus, the main contribution to Y_1 is provided by n_Q and ℓ with $\frac{n_Q}{\ell} = \Theta\left(n^{4/3}m_U^{-2/3}\right)$. Combining that together with Lemma 13 we get

$$\frac{\upsilon_1(n_Q+1,\ell)}{\upsilon_1(n_Q,\ell)} = \exp\left(O\left(n^{-2/3}\right) - \Theta(1)\left(1-\frac{2m_U}{n_U}\right)^2\right).$$

Thus, the main contribution to Y_1 is provided by n_Q and ℓ with $\frac{n_Q+2\ell-2s}{n_U} = \left(1-\frac{2m_U}{n_U}\right) = O_p\left(n^{-1/3}\right)$, which yields $n_Q+2\ell-2s = O_p\left(n^{2/3}\right)$. Together with $\frac{n_Q}{\ell} = \Theta\left(n^{4/3}m_U^{-2/3}\right)$ this implies $n_Q = 2s + O_p\left(n^{2/3}\right)$ and $\ell = \Theta\left(sn^{-2/3}\right)$. ◀

Proof of Lemma 19. We define

$$\upsilon_2(n_Q,\ell) := \binom{n}{n_Q}|\mathcal{Q}(n_Q,n_Q+\ell)|\binom{\binom{n_U}{2}}{m_U}c\left(\frac{2}{e}\right)^{2m_U-n_U}\frac{m_U^{m_U+1/2}n_U^{n_U-2m_U+g(n_Q)}}{(n_U-m_U)^{n_U-m_U+1/2}},$$

where $c>0$, $h(n)=\omega(1)$ and $g(n_Q) := \frac{1}{2}$ if $n_Q \leq 2s - n^{2/3}h(n)$ and $g(n_Q) := 0$ otherwise. By Lemma 12 we can choose $h(n)$ and c so that for all admissible n_Q and ℓ, we have $\tau(n_Q,\ell) \leq \upsilon_2(n_Q,\ell)$. Similarly as in the proof of Lemma 18 we obtain that the main contribution to $Y_2 := \sum_{n_U<2m_U}\upsilon_2(n_Q,\ell)$ is provided by $n_Q = 2s + O_p\left(n^{2/3}\right)$ and $\ell = \Theta\left(sn^{-2/3}\right)$. For such n_Q and ℓ we have $g(n_Q)=0$ and by Lemma 12(ii) $|\mathcal{U}(n_U,m_U)| = \Theta_p(1)\binom{\binom{n_U}{2}}{m_U}$. Using that we obtain $\frac{\upsilon_2(n_Q,\ell)}{\tau(n_Q,\ell)} = \Theta_p(1)$, which shows the statement. ◀

Proof of Lemma 21. Let $\widetilde{n} = n_Q - |H_1(Q_G)|$ and we look at the following operation in G. We add an edge between two different complex components and delete an edge in a non-complex component. We have whp $\Omega\left(s\widetilde{n}n\right)$ choices for performing this operation. We observe that in the reverse operation we delete an edge from the core and add some edge. We can do that whp in $O\left(sn^{-1/3}n^2\right)$ different ways. Hence, it follows that $\widetilde{n} = O_p\left(\frac{sn^{5/3}}{sn}\right) = O_p\left(n^{2/3}\right)$. ◀

Proof of Lemma 22. Let $H \in \mathcal{A}(n,m)$ be a graph that has a vertex lying in three blocks. We consider the following operation in the core C_H:

- We choose a vertex x that lies in three blocks;
- Let X be the component of C_H containing x. Then we choose a component Y of $X-x$ that contains at most $n_C(H)/3$ vertices, but two neighbours of x (in H);
- We choose a vertex y in C_H which is not in Y and has degree two;
- For all neighbours z of x in Y we delete the edge xz and insert the edge yz.

We observe that we have at least $2n_C(H)/3 - 2\ell = \Theta\left(sn^{-1/3}\right)$ options for performing this operation. On the other hand, we note that in a constructed graph H' the following holds:

- $H' \in \mathcal{A}(n,m)$, $n_C(H') = n_C(H)$ and $\ell(H') = \ell(H)$;
- y lies in one or two blocks and has at least degree four;
- x has at least degree four.

Hence, a fixed graph H' can be constructed in at most $2\ell \cdot 2 \cdot 2\ell = \Theta\left(s^2 n^{-4/3}\right)$ many different ways. Now the statement follows, since $\Theta\left(\frac{s^2 n^{-4/3}}{sn^{-1/3}}\right) = o(1)$. ◀

Proof of Lemma 23. We consider the kernel K_H of a graph $H \in \mathcal{A}(n,m)$ which has a chord. Then K_H has a chord xy with the following property: If B' is the unique Hamiltonian cycle of the block B containing x and y, then there is a path $z_0 = x, z_1, \ldots, z_{t+1} = y$ in B' such that there is no chord in B containing one of the vertices $z_1, \ldots, z_t$. Next, we choose a random core which can be obtained by subdividing the edges of K_H which are not chords by $n_C(H) - |K_H|$ additional vertices. We denote by X the number of vertices which subdivide the edge $z_0 z_1$. Using a "bins and balls" type argument, we can show that $\mathbb{P}[X = j] \leq \mathbb{P}[X = 0]$ for any $j \in \mathbb{N}$ and $\mathbb{P}[X = 0] = O\left(\frac{|K_H|}{n_C(H) - |K_H|}\right) = O\left(n^{-1/3}\right)$. Thus, $\mathbb{P}\left[X \leq n^{1/3} h(n)^{-1}\right] \leq \left(n^{1/3} h(n)^{-1} + 1\right) \mathbb{P}[X = 0] = o(1)$, i.e. whp $z_0 z_1$ is subdivided by at least $n^{1/3} h(n)^{-1} + 1$ vertices, which shows the statement. ◀

7 Concluding remarks

Kang, Moßhammer, and Sprüssel [13] showed that graphs on orientable surfaces feature a second phase transition at $m = n + O\left(n^{3/5}\right)$, where the number of vertices outside the largest component becomes sublinear. By Theorem 3 and Remark 8.6 in [13] this is also true for random cactus graphs. Thus, we believe that this should also be the case for random outerplanar graphs, since the class of outerplanar graphs lies "between" the class of cactus graphs and the class of graphs on orientable surfaces. Unfortunately, our method does not seem to work when $m = n + o(n)$. This is mainly because the bound in Lemma 16 is not good enough in that regime.

Theorem 4 raises the following question. How does the probability that $A(n,m)$ is a cactus graph behave if m grows? By looking at the proof of Theorem 4 a natural guess would be the following.

▶ **Conjecture 24.** *If $m = \alpha n$ for $1/2 < \alpha < 1$, then the probability that $A(n,m)$ is a cactus graph is bounded away from 0 and 1.*

▶ **Conjecture 25.** *If $m = n + t$ for $t = o(n)$, then whp $A(n,m)$ is not a cactus graph.*

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A An application of Lemma 8: proof of Lemma 10

To illustrate how to apply Lemma 8 we prove Lemma 10 in this section (the proof of Lemma 11 is similar). We start by getting an upper bound for $\frac{\rho(n_C)}{\rho(n_C+1)}$. By Lemma 9(i) we obtain

$$\begin{aligned}
\frac{\rho\left(n_C\right)}{\rho(n_C+1)} &= \frac{n_C+1}{n_Q-n_C}\cdot\frac{n_Cn_Q}{n_C+1}\cdot\frac{|\mathcal{C}(n_C,n_C+\ell)|}{|\mathcal{C}(n_C+1,n_C+1+\ell)|}\\
&\le \frac{n_Cn_Q}{n_Q-n_C}\frac{1}{n_C+\frac{\ell}{80}}\\
&= \left(1-\frac{\ell}{80n_C+\ell}\right)\left(1+\frac{n_C}{n_Q-n_C}\right)\\
&\le \exp\left(-\frac{\ell}{80n_C+\ell}+\frac{n_C}{n_Q-n_C}\right).
\end{aligned}$$

Next, we observe that $\ell\le n_C\le n_Q$, since an outerplanar graph on n_C vertices can have at most $2n_C$ edges. Hence, we can choose $c>0$ small enough such that for all $n_C\le 2c\sqrt{n_Q\ell}$

$$\begin{aligned}
\frac{\rho\left(n_C\right)}{\rho(n_C+1)} &\le \exp\left(-\frac{\ell}{81n_C}+\frac{2n_C}{n_Q}\right)\\
&\le \exp\left(-\frac{\ell}{81\cdot 2c\sqrt{n_Q\ell}}+\frac{2\cdot 2c\sqrt{n_Q\ell}}{n_Q}\right)\\
&\le \exp\left(-\sqrt{\frac{\ell}{n_Q}}\right)=\exp\left(h(n)\right),
\end{aligned}$$

where $h(n) := -\sqrt{\frac{\ell}{n_Q}}$. We also define $g(n) := c\sqrt{n_Q \ell}$ and $f_n(n_C) := n_C + g(n)$. Then we obtain for all $n_C \le c\sqrt{n_Q \ell}$

$$\frac{\rho(n_C)}{\rho(f_n(n_C))} = \prod_{k=n_C}^{f_n(n_C)-1} \frac{\rho(k)}{\rho(k+1)} \le \exp(h(n))^{g(n)} = \exp(-c\ell).$$

Finally, that yields

$$\sum_{n_C \le c\sqrt{n_Q \ell}} \rho(n_C) \le \exp(-c\ell) \sum_{n_C \le c\sqrt{n_Q \ell}} \rho(f_n(n_C)) \le \exp(-c\ell) \sum_{n_C} \rho(n_C),$$

which shows the statement.
We conclude this section by observing an immediate consequence of Lemma 10. Assuming $\ell = \omega(1)$, which is true due to Lemmas 18 and 19, we have $\frac{\rho(n_C)}{\rho(f_n(n_C))} \le \exp(-c\ell) = o(1)$. Then Lemma 8 implies that the terms provided by $I_1(n) := \left\{n_C \mid n_C \le c\sqrt{n_Q \ell}\right\}$ are negligible in $\sum_{n_C} \rho(n_C)$.

B Proof of Lemma 14

We shall focus on the proof of the lower bound, since the upper bound can be shown in a similar way. We will use the core-kernel approach from [13] and recall that $\mathcal{T}$ is the class of all cactus graphs. Then we denote by $\mathcal{C}_C$ the class of all cores of graphs in $\mathcal{T}$ and by $\mathcal{K}_C$ the class of all kernels of graphs in $\mathcal{T}$. Analogously to (2) we obtain

$$|\mathcal{Q}_C(n_Q, n_Q + \ell)| = \sum\nolimits_{n_C} \binom{n_Q}{n_C} |\mathcal{C}_C(n_C, n_C + \ell)| n_C n_Q^{n_Q - n_C - 1}. \tag{12}$$

We claim that

$$|\mathcal{C}_C(n_C, n_C + \ell)| \ge \binom{n_C}{2\ell} |\mathcal{K}_C(2\ell, 3\ell)| (n_C - 2\ell)! \binom{n_C - 5\ell - 1}{3\ell - 1}. \tag{13}$$

Indeed, we can construct (not necessarily all) graphs from $\mathcal{C}_C(n_C, n_C + \ell)$ in the following way. We choose 2ℓ labels from $[n_C]$ for the vertices of the kernel. Then we pick a kernel K from $\mathcal{K}_C(2\ell, 3\ell)$ and assign the labels chosen before to the vertices of K. Finally, we subdivide the edges of the kernel by the $(n_C - 2\ell)$ remaining vertices such that each edge is subdivided by at least two vertices, which guarantees that the obtained graph is simple. Thus, all constructed graphs are in $\mathcal{C}_C(n_C, n_C + \ell)$. We note that there are $w(K)\,(n_C - 2\ell)!\binom{n_C - 5\ell - 1}{3\ell - 1}$ many ways to get such a subdivision, where $w(K) = 2^{-e_1(K) - e_2(K)}$ and $e_1(K)$ denotes the number of loops in K and $e_2(K)$ the number of double edges in K. In addition, we note that in $|\mathcal{K}_C(2\ell, 3\ell)|$ each kernel K is counted with a weight of $w(K)$. Then inequality (13) follows by the aforementioned construction. Combining (12) and (13) we obtain

$$\begin{aligned} |\mathcal{Q}_C(n_Q, n_Q + \ell)| &\ge \frac{|\mathcal{K}_C(2\ell, 3\ell)|\, n_Q^{n_Q - 1}}{(2\ell)!(3\ell - 1)!} \sum\nolimits_{n_C} (n_Q)_{n_C} (n_C - 5\ell - 1)_{3\ell - 1}\, n_C n_Q^{-n_C} \\ &= \frac{|\mathcal{K}_C(2\ell, 3\ell)|\, n_Q^{n_Q - 1}}{(2\ell)!(3\ell - 1)!} \sum\nolimits_{n_C} \nu(n_C), \end{aligned} \tag{14}$$

where $\nu(n_C) := (n_Q)_{n_C} (n_C - 5\ell - 1)_{3\ell - 1}\, n_C n_Q^{-n_C}$. Next, we observe that

$$\frac{\nu(n_C + 1)}{\nu(n_C)} = \frac{n_Q - n_C}{n_Q} \frac{n_C - 5\ell}{n_C - 8\ell + 1} \frac{n_C + 1}{n_C}.$$

We note that $\frac{\nu(n_C+1)}{\nu(n_C)}$ is decreasing in n_C and that $\frac{\nu(\overline{n_C}+1)}{\nu(\overline{n_C})} \approx 1$ for $\overline{n_C} = \sqrt{3n_Q\ell}$. Thus, we expect that we obtain a good approximation for $\sum_{n_C} \nu(n_C)$ by considering only terms whose index is "close" to $\overline{n_C}$. In the following we make that more precise. We note that for $\ell \le \varepsilon n_Q$ and $\varepsilon > 0$ small enough, we get

$$\nu\left(\overline{n_C}\right) \ge \left(1 - \frac{\sqrt{3n_Q\ell}}{n_Q}\right)^{\sqrt{3n_Q\ell}} \left(\sqrt{3n_Q\ell} - 8\ell\right)^{3\ell} \ge \exp\left(-6\ell\right) \sqrt{n_Q\ell}^{3\ell}. \tag{15}$$

Next, we distinguish two cases. First we assume $\ell \le \sqrt{n_Q}$. Then we get for all $n_C \ge \overline{n_C} - \sqrt{n_Q}$ and $\varepsilon > 0$ small enough

$$\begin{aligned}
\frac{\nu(n_C+1)}{\nu\left(n_C\right)} &\le \left(1 - \frac{n_C}{n_Q}\right)\left(1 + \frac{3\ell}{n_C - 8\ell}\right)\left(1 + \frac{1}{n_C}\right) \\
&\le \exp\left(-\sqrt{\frac{3\ell}{n_Q}} + \frac{3\ell}{\sqrt{3n_Q\ell} - \sqrt{n_Q} - 8\ell} + \frac{3}{\sqrt{n_Q}}\right) \\
&\le \exp\left(\sqrt{\frac{3\ell}{n_Q}} \cdot \frac{27\sqrt{n_Q}}{\sqrt{3n_Q\ell}} + \frac{3}{\sqrt{n_Q}}\right) = \exp\left(\frac{30}{\sqrt{n_Q}}\right).
\end{aligned}$$

Hence, we obtain $\nu\left(n_C\right) \ge \nu\left(\overline{n_C}\right)\exp(-30)$ for all $\overline{n_C} - \sqrt{n_Q} \le n_C \le \overline{n_C}$. Combining that together with (14), (15) and Theorem 3 yields

$$\begin{aligned}
\left|\mathcal{Q}_C(n_Q, n_Q+\ell)\right| &\ge \frac{\left|\mathcal{K}_C(2\ell,3\ell)\right| n_Q^{n_Q-1}}{(2\ell)!(3\ell-1)!}\sqrt{n_Q}\nu\left(\overline{n_C}\right)\exp(-30) \\
&\ge \Theta(1)^\ell n_Q^{n_Q+3\ell/2-1/2}\ell^{3\ell/2-5/2-3\ell+1/2} \\
&= \Theta(1)^\ell n_Q^{n_Q+3\ell/2-1/2}\ell^{-3\ell/2-2},
\end{aligned}$$

which shows the statement for the case $\ell \le \sqrt{n_Q}$. Finally, we assume $\ell > \sqrt{n_Q}$. Then we get by (14), (15) and Theorem 3 for $\varepsilon > 0$ small enough

$$\begin{aligned}
\left|\mathcal{Q}_C(n_Q, n_Q+\ell)\right| &\ge \frac{\left|\mathcal{K}_C(2\ell,3\ell)\right| n_Q^{n_Q-1}}{(2\ell)!(3\ell-1)!}\nu\left(\overline{n_C}\right) \\
&\ge \Theta(1)^\ell n_Q^{n_Q-1+3\ell/2}\ell^{3\ell/2-5/2-3\ell+1/2} \\
&= \Theta(1)^\ell n_Q^{n_Q+3\ell/2-1/2}\ell^{-3\ell/2-2}n_Q^{-1/2} \\
&\ge \Theta(1)^\ell n_Q^{n_Q+3\ell/2-1/2}\ell^{-3\ell/2-2}\exp\left(-\sqrt{\frac{\ell^3}{n_Q}}\right),
\end{aligned}$$

as desired.

Probabilistic Analysis of Optimization Problems on Sparse Random Shortest Path Metrics

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Abstract

Simple heuristics for (combinatorial) optimization problems often show a remarkable performance in practice. Worst-case analysis often falls short of explaining this performance. Because of this, "beyond worst-case analysis" of algorithms has recently gained a lot of attention, including probabilistic analysis of algorithms.

The instances of many (combinatorial) optimization problems are essentially a discrete metric space. Probabilistic analysis for such metric optimization problems has nevertheless mostly been conducted on instances drawn from Euclidean space, which provides a structure that is usually heavily exploited in the analysis. However, most instances from practice are not Euclidean. Little work has been done on metric instances drawn from other, more realistic, distributions. Some initial results have been obtained in recent years, where random shortest path metrics generated from dense graphs (either complete graphs or Erdős–Rényi random graphs) have been used so far.

In this paper we extend these findings to sparse graphs, with a focus on grid graphs. A random shortest path metric is constructed by drawing independent random edge weights for each edge in the graph and setting the distance between every pair of vertices to the length of a shortest path between them with respect to the drawn weights. For such instances generated from a grid graph, we prove that the greedy heuristic for the minimum distance maximum matching problem, and the nearest neighbor and insertion heuristics for the traveling salesman problem all achieve a constant expected approximation ratio. Additionally, for instances generated from an arbitrary sparse graph, we show that the 2-opt heuristic for the traveling salesman problem also achieves a constant expected approximation ratio.

2012 ACM Subject Classification Mathematics of computing → Approximation algorithms; Mathematics of computing → Combinatorial optimization; Theory of computation → Approximation algorithms analysis; Theory of computation → Random network models

Keywords and phrases Random shortest paths, Random metrics, Approximation algorithms, First-passage percolation

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.19

Funding This research was supported by NWO grant 613.001.402.

1 Introduction

Large-scale optimization problems, such as the traveling salesman problem (TSP), are relevant for many applications. Often it is not possible to solve these problems to optimality within a reasonable amount of time, especially when instances get larger. Therefore, in practice these kind of problems are tackled by using approximation algorithms or ad-hoc heuristics. Even though the worst-case performance of these, often simple, heuristics is usually rather bad, they often show a remarkably good performance in practice.

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 19; pp. 19:1–19:16
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

In order to find theoretical results that are closer to the practical observations, probabilistic analysis has been a useful tool over the last decades. One of the main challenges here is to choose a probability distribution on the set of possible instances of the problem: on the one hand this distribution should be sufficiently simple in order to make the probabilistic analysis possible, but on the other hand the distribution should somehow reflect realistic instances.

In the "early days" of probabilistic analysis, random instances were either generated by using independent random edge lengths or embedded in Euclidean space (e.g. [2, 11]). Although these models have some nice mathematical properties that enable the probabilistic analysis, they have shortcomings regarding their realism: in practice, instances are often metric, but not Euclidean, and independent random edge lengths are not even metric.

Recently, Bringmann et al. [6] widened the scope of models for generating random instances by using the following model, already proposed by Karp and Steele in 1985 [17]: given an undirected complete graph, draw edge weights independently at random and then define the distance between any two vertices as the total weight of the shortest path between them, measured with respect to those random weights. Even though this model broadens the scope of random metric spaces, the resulting instances from this model are not very realistic.

In this paper we adapt this model in the sense that we start with a sparse graph instead of a complete graph. We believe that this yields instances that are more realistic, for instance since in practice the underlying (road, communication, etc.) networks are almost always sparse.

Related Work

The model described above is known by two different names: *random shortest path metrics* and *first-passage percolation*. It was introduced by Hammersley and Welsh under the latter name as a model for fluid flow through a (random) porous medium [12, 14]. A lot of studies have been conducted on first-passage percolation, mostly on this model defined on the lattice $\mathbb{Z}^d$.

For first-passage percolation on complete graphs many structural results exist. We know for instance that the expected distance between two arbitrary fixed vertices is approximately $\ln(n)/n$ and that the distance from a fixed vertex to the vertex that is farthest away from it is approximately $2\ln(n)/n$ [6, 15]. We also know that the diameter in this case is approximately $3\ln(n)/n$ [13, 15]. Bringmann et al. used this model to analyze heuristics for matching, TSP and k-median [6].

There has been a lot of interest in first-passage percolation on the integer lattice $\mathbb{Z}^d$. Although very few precise results are known for this model, there are many existential results available. For instance, the distance between the origin and $n\mathbf{e}_1$ (where $\mathbf{e}_1$ is the unit vector in the first coordinate direction) is known to be $\Theta(n)$ [12]. Also, the set of vertices within distance t from the origin grows linearly in t and, after rescaling, converges to some convex domain [20]. The survey by Auffinger et al. [1] contains a thorough overview.

Our Results

This paper aims at extending the results of Bringmann et al. [6] and Klootwijk et al. [18] to the more realistic setting of random shortest path metrics generated from sparse graphs. For simplicity, most of the results in this paper assume that these sparse graphs are (finite square) grid graphs. We believe that the probabilistic analysis of simple heuristics in different random models will enhance the understanding of the performance of these heuristics, which are used in many applications.

In this paper we consider two different types of simple heuristics. In Section 4 we conduct a probabilistic analysis of three greedy-like heuristics: the greedy heuristic for the minimum-distance perfect matching problem, and the nearest neighbor heuristic and insertion heuristic for the TSP. In Section 5 we conduct a probabilistic analysis of a local search heuristic: the 2-opt heuristic for the TSP. We show that all four heuristics yield a constant approximation ratio for random shortest path metrics generated from (finite square) grid graphs (greedy-like in Section 4) or arbitrary sparse graphs (local search in Section 5). We are aware that our results are mostly purely theoretical, because, e.g., cheapest insertion already achieves an approximation ratio of 2 and is often used to initialize 2-opt [10, 21]. However, they are non-trivial results about practically used algorithms, beyond the classical worst-case analysis.

2 Notation and Model

For $n \in \mathbb{N}$, we use $[n]$ as shorthand notation for $\{1, \dots, n\}$. Sometimes we use $\exp(\cdot)$ to denote the exponential function. We denote by $X \sim P$ that a random variable X is distributed according to a probability distribution P, where in particular $\operatorname{Exp}(\lambda)$ denotes the exponential distribution with parameter λ. We write $X \sim \sum_{i=1}^{n} \operatorname{Exp}(\lambda_i)$ if X is the sum of n independent exponentially distributed random variables having parameters $\lambda_1, \dots, \lambda_n$. In particular, $X \sim \sum_{i=1}^{n} \operatorname{Exp}(\lambda)$ denotes an Erlang distribution with parameters n and λ. If a random variable X_1 is stochastically dominated by a random variable X_2, i.e., we have $F_1(x) \geq F_2(x)$ for all x (where F_i is the distribution function of X_i), we denote this by $X_1 \precsim X_2$.

Random Shortest Path Metrics

Given an undirected connected graph $G = (V, E)$, the corresponding random shortest path metric is constructed as follows. First, for each edge $e \in E$, draw a random edge weight $w(e)$ independently according to the exponential distribution with parameter 1. (Exponential distributions are technically easiest to handle since they are memoryless.) Then, define the distance function $d : V \times V \to \mathbb{R}_{\geq 0}$ as follows: for each $u, v \in V$, $d(u, v)$ is the total weight of a lightest u,v-path in G (w.r.t. to the random weights $w(\cdot)$). Observe that this definition immediately implies that $d(v, v) = 0$ for all $v \in V$, that $d(u, v) = d(v, u)$ for all $u, v \in V$, and that $d(u, v) \leq d(u, s) + d(s, v)$ for all $u, s, v \in V$. We call the distance function d obtained by this process a random shortest path metric generated from G.

We use the following notation to denote properties of these random shortest path metrics. $\Delta_{\max} := \max_{u,v} d(u, v)$ denotes the diameter of the random metric. The Δ-ball around a vertex v, $B_\Delta(v) := \{u \in V \mid d(u, v) \leq \Delta\}$, is the set of vertices within distance Δ of v. Let $\pi_k(v)$ denote the kth closest vertex from v (including v itself and breaking ties arbitrarily). Note that $v = \pi_1(v)$ for all $v \in V$. The distance from a vertex v to this kth closest vertex from it is denoted by $\tau_k(v) := d(v, \pi_k(v)) = \min\{\Delta \mid |B_\Delta(v)| \geq k\}$. Slightly abusing notation, we let $B_{\tau_k(v)}(v) := \{\pi_i(v) \mid i = 1, \dots, k\}$ denote the set of the k closest vertices to v (including v itself). The size of the cut in G induced by this set, which plays an important role in our analysis, is denoted by $\chi_k(v) := |\delta(B_{\tau_k(v)}(v))|$, where $\delta(U) := \{\{u, v\} \in E \mid u \in U, v \notin U\}$ denotes the cut induced by U.

During our analysis in Sections 4 and 5 it is convenient to describe (partial) solutions to the minimum-distance perfect matching problem and the TSP as sets of "edges". In order to emphasize that such "edges" in principle do not coincide with edges from G, we use quotation marks to distinguish them.

Sparse Graphs

Throughout this paper, G is a sparse connected undirected simple graph on n vertices, i.e., we have $|E| = \Theta(|V|) = \Theta(n)$. Most of the results in this paper are restricted to a specific class of sparse graphs, namely the finite square grid graph. This graph has vertex set $V = [N]^2$, and two vertices $(x_1, y_1), (x_2, y_2) \in V$ are connected if and only if $|x_1 - x_2| + |y_1 - y_2| = 1$. It is easy to see that for these graphs we have $|V| = n = N^2$ and $|E| = 2N^2 - 2N = \Theta(n)$.

For practical reasons we assume in this paper that n is even. Note that the results concerning the minimum-distance perfect matching problem are only valid when n is even. All results concerning the travelling salesman problem can easily be extended to odd n.

3 Structural Properties

In this section, we provide some structural properties regarding sparse random shortest path metrics that are used later on in our probabilistic analyses of the greedy heuristic for maximum matching and the 2-opt heuristic for the TSP in such random metric spaces. We start of with some technical lemmas from known literature and some results regarding sums of lightest edge weights in G (which hold for arbitrary sparse graphs). After that, we consider a random growth process that is closely related to the special case of random shortest path metrics generated from a finite square grid graph and use it to derive a clustering result and a tail bound on the diameter $\Delta_{\max}$.

Technical Lemmas

▶ **Lemma 1** ([16, Thm. 5.1(i,iii)]). *Let $X \sim \sum_{i=1}^{m} \mathrm{Exp}(a_i)$. Let $\mu = \mathbb{E}[X] = \sum_{i=1}^{m} 1/a_i$ and $a_* = \min_i a_i$.*

(i) *For any $\lambda \geq 1$,*

$$\mathbb{P}\left(X \geq \lambda\mu\right) \leq \lambda^{-1} \exp\left(-a_*\mu\left(\lambda - 1 - \ln(\lambda)\right)\right).$$

(iii) *For any $\lambda \leq 1$,*

$$\mathbb{P}\left(X \leq \lambda\mu\right) \leq \exp\left(-a_*\mu\left(\lambda - 1 - \ln(\lambda)\right)\right).$$

▶ **Corollary 2.** *Let $X \sim \sum_{i=1}^{m} \mathrm{Exp}(a_i)$. Let $\mu = \mathbb{E}[X] = \sum_{i=1}^{m} 1/a_i$ and $a_* = \min_i a_i$. For any x,*

$$\mathbb{P}\left(X \leq x\right) \leq \exp\left(a_*\mu\left(1 + \ln(x/\mu)\right)\right).$$

Proof. Let $\lambda := x/\mu$. If $\lambda \leq 1$, the result is a weaker version of Lemma 1(iii). If $\lambda > 1$, then $1 + \ln(x/\mu) > 0$ and hence $\mathbb{P}(X \leq x) \leq 1 < \exp(a_*\mu(1 + \ln(x/\mu)))$. ◀

▶ **Lemma 3** ([5, Thm. 2(ii)]). *Let $X \sim \sum_{i=1}^{m} \mathrm{Exp}(\lambda_i)$ and $Y \sim \sum_{i=1}^{m} \mathrm{Exp}(\eta)$. Then*

$$X \succsim Y \qquad \text{if and only if} \qquad \prod_{i=1}^{m} \lambda_i \leq \eta^m.$$

Sums of Lightest Edge Weights in G

All main results in this paper make use of some observations relating sums of the m lightest edge weights in a sparse graph G. The lemmas and corollary below summarize some structural properties concerning these sums. They hold for arbitrary sparse graphs G.

▶ **Lemma 4.** *Let S_m denote the sum of the m lightest edge weights in G. Then*

$$\sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{e|E|}{m}\right) \precsim S_m \precsim \sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{|E|}{m}\right).$$

Proof. Let σ_k denote the kth lightest edge weight in G. Since all edge weights are independent and standard exponentially distributed, we have $\sigma_1 = S_1 \sim \mathrm{Exp}(|E|)$. Using the memorylessness property of the exponential distribution, it follows that $\sigma_2 \sim \sigma_1 + \mathrm{Exp}(|E|-1)$, i.e., the second lightest edge weight is equal to the lightest edge weight plus the minimum of $|E|-1$ standard exponential distributed random variables. In general, we get $\sigma_{k+1} \sim \sigma_k + \mathrm{Exp}(|E|-k)$. The definition $S_m = \sum_{k=1}^{m} \sigma_k$ yields

$$S_m \sim \sum_{i=0}^{m-1} (m-i) \cdot \mathrm{Exp}\left(|E|-i\right) \sim \sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{|E|-i}{m-i}\right).$$

Now, the first stochastic dominance relation follows from Lemma 3 by observing that

$$\prod_{i=0}^{m-1} \frac{|E|-i}{m-i} = \frac{|E|!}{m!(|E|-m)!} = \binom{|E|}{m} \le \left(\frac{e|E|}{m}\right)^m,$$

where the inequality follows from applying the well-known inequality $\binom{n}{k} \le (en/k)^k$. The second stochastic dominance relation follows by observing that $|E| \ge m$, which implies that $(|E|-i)/(m-i) \ge |E|/m$ for all $i = 0, \ldots, m-1$. ◀

▶ **Corollary 5.** *Let S_m denote the sum of the m lightest edge weights in G. Then $\mathbb{E}[S_m] = \Theta(m^2/n)$.*

Proof. From Lemma 4 we can immediately see that

$$\mathbb{E}\left[\sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{e|E|}{m}\right)\right] \le \mathbb{E}\left[S_m\right] \le \mathbb{E}\left[\sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{|E|}{m}\right)\right].$$

The result follows by observing that

$$\mathbb{E}\left[\sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{e|E|}{m}\right)\right] = \frac{m^2}{e|E|} \quad \text{and} \quad \mathbb{E}\left[\sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{|E|}{m}\right)\right] = \frac{m^2}{|E|},$$

and recalling that $|E| = \Theta(n)$ by our restrictions imposed on G. ◀

▶ **Lemma 6.** *Let S_m denote the sum of the m lightest edge weights in G. Then we have*

$$\mathbb{P}\left(S_m \le cn\right) \le \exp\left(m\left(2 + \ln\left(\frac{c|E|n}{m^2}\right)\right)\right).$$

Proof. First of all, Lemma 4 yields

$$S_m \succsim \sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{e|E|}{m}\right).$$

Now, we apply Corollary 2 with $\mu = m^2/e|E|$, $a_* = e|E|/m$, and $x = cn$ to obtain

$$\mathbb{P}\left(S_m \le cn\right) \le \mathbb{P}\left(\sum_{i=0}^{m-1} \mathrm{Exp}\left(\frac{e|E|}{m}\right) \le cn\right) \le \exp\left(m\left(1 + \ln\left(\frac{ce|E|n}{m^2}\right)\right)\right).$$

The result follows immediately. ◀

▶ **Lemma 7.** *Let S_m denote the sum of the m lightest edge weights in G. Then we have* $\mathsf{TSP} \geq \mathsf{MM} \geq S_{n/2}$*, where* TSP *and* MM *are the total distance of a shortest TSP tour and a minimum-distance perfect matching, respectively.*

Proof. The first inequality is trivial. For the second one, consider a minimum-distance perfect matching in G, and take the union of the shortest paths between each pair of matched vertices. This union H must contain at least $n/2$ different edges of G, since H is a forest with n vertices, all of which are non-isolated in H. These $n/2$ different edges together have a weight of at least $S_{n/2}$ and at most MM. So, the second inequality follows. ◀

A Random Growth Process

In this subsection, and the following ones, we assume that G is a finite square grid graph with $n = N^2$ vertices. It is possible to obtain qualitatively similar results for more general classes of sparse graphs, but in order to improve readability we chose to stick with grid graphs.

In order to understand sparse random shortest path metrics it is important to get a feeling for the distribution $\tau_k(v)$. However, this distribution depends heavily on the exact position of v within G, which makes it rather complicated to derive it. In order to overcome this, we derive instead a stochastic upper bound on $\tau_k(v)$ which holds for any vertex $v \in V$. The following lemma and corollary establish this.

▶ **Lemma 8** ([4, Thm. 3])**.** *Let $U \subseteq V$. Then we have*

$$|\delta(U)| \geq \begin{cases} 2\sqrt{|U|} & \text{if } |U| \leq n/4, \\ \sqrt{n} & \text{if } n/4 \leq |U| \leq 3n/4, \\ 2\sqrt{n - |U|} & \text{if } |U| \geq 3n/4. \end{cases}$$

▶ Remark. Bollobás and Leader [4] proved (a more general version of) this result for all $|U| \leq n/2$. The result for $|U| > n/2$ follows immediately from their result by observing that $\delta(U) = \delta(V \backslash U)$ and $|V \backslash U| = n - |U|$ for all $U \subseteq V$.

▶ **Corollary 9.** *For any $v \in V$ and any $k \leq n/4$ we have*

$$\tau_k(v) \precsim \sum_{i=1}^{k-1} \mathrm{Exp}(2\sqrt{i}).$$

Proof. The values of $\tau_k(v)$ are generated by a birth process as follows. (Similar birth processes have been analysed before (e.g. [6, 8, 18]).) For $k = 1$ we have $\tau_k(v) = 0$ and also $\sum_{i=1}^{k-1} \mathrm{Exp}(2\sqrt{i}) = 0$. For $k \geq 2$, we can obtain $\tau_k(v)$ from $\tau_{k-1}(v)$ by looking at all edges that "leave" $B_{\tau_{k-1}(v)}(v)$, i.e., edges (u, x) with $u \in B_{\tau_{k-1}(v)}(v)$ and $x \notin B_{\tau_{k-1}(v)}(v)$. By definition there are $\chi_{k-1}(v)$ such edges, and from Lemma 8 it follows that $\chi_{k-1}(v) \geq 2\sqrt{k-1}$ (since $k \leq n/4$). Moreover, by definition of $\tau_{k-1}(v)$ these edges are conditioned to have a length of at least $\tau_{k-1}(v) - d(v, u)$. Using the memorylessness of the exponential distribution, it follows that $\tau_k(v) - \tau_{k-1}(v)$ is the minimum of $\chi_{k-1}(v)$ exponential random variables (with parameter 1), or, equivalently, $\tau_k(v) - \tau_{k-1}(v) \sim \mathrm{Exp}(\chi_{k-1}(v)) \precsim \mathrm{Exp}(2\sqrt{k-1})$), where the stochastic dominance follows since $\chi_{k-1}(v) \geq 2\sqrt{k-1}$. The result follows by induction. ◀

Now we use this stochastic upper bound on $\tau_k(v)$ that holds for any $v \in V$ to derive some bounds on the cumulative distribution functions of $\tau_k(v)$ and $|B_\Delta(v)|$. The final bound is a crucial ingredient for the construction of clusterings in the next section.

▶ **Lemma 10.** *For any $\Delta > 0$, $v \in V$, and $k \in [n]$ such that $k \leq \min\{n/4, \Delta^2 + 1\}$, we have*

$$\mathbb{P}\left(\tau_k(v) \leq \Delta\right) \geq 1 - \frac{\sqrt{k-1}}{\Delta} \cdot \exp\left(-2(\sqrt{k}-1)\left(\frac{\Delta}{\sqrt{k-1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{k-1}}\right)\right)\right).$$

Proof. From Corollary 9 we can see that

$$\mathbb{P}\left(\tau_k(v) \leq \Delta\right) \geq \mathbb{P}\left(\sum_{i=1}^{k-1} \mathrm{Exp}(2\sqrt{i}) \leq \Delta\right) = 1 - \mathbb{P}\left(\sum_{i=1}^{k-1} \mathrm{Exp}(2\sqrt{i}) \geq \Delta\right).$$

Next, we want to apply the result of Lemma 1(i). For this purpose, set

$$\mu := \mathbb{E}\left[\sum_{i=1}^{k-1} \mathrm{Exp}(2\sqrt{i})\right] = \sum_{i=1}^{k-1} \frac{1}{2\sqrt{i}} \qquad \text{and} \qquad \lambda := \frac{\Delta}{\mu},$$

and observe that $\sqrt{k} - 1 \leq \mu \leq \sqrt{k-1}$. Also note that $\lambda = \Delta/\mu \geq \Delta/\sqrt{k-1} \geq 1$ since $k \leq \Delta^2 + 1$. Lemma 1(i) now yields

$$1 - \mathbb{P}\left(\sum_{i=1}^{k-1} \mathrm{Exp}(2\sqrt{i}) \geq \Delta\right) \geq 1 - \lambda^{-1} \exp\left(-2\mu(\lambda - 1 - \ln(\lambda))\right).$$

It can now be seen that this final expression is increasing in both μ and λ. Therefore, we may apply the inequalities $\mu \geq \sqrt{k} - 1$ and $\lambda \geq \Delta/\sqrt{k-1}$ to obtain the desired result. ◀

▶ **Lemma 11.** *For any $\Delta > 0$, $v \in V$, and $k \in [n]$ such that $k \leq \min\{n/4, \Delta^2 + 1\}$, we have*

$$\mathbb{P}\left(|B_\Delta(v)| \geq k\right) \geq 1 - \frac{\sqrt{k-1}}{\Delta} \cdot \exp\left(-2(\sqrt{k}-1)\left(\frac{\Delta}{\sqrt{k-1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{k-1}}\right)\right)\right).$$

Proof. This lemma follows immediately from Lemma 10 by observing that $|B_\Delta(v)| \geq k$ if and only if $\tau_k(v) \leq \Delta$. ◀

▶ **Corollary 12.** *Let $n \geq 9$. There exists a constant $c_1 \geq 4$ such that for any $\Delta > 0$ and $v \in V$ we have*

$$\mathbb{P}\left(|B_\Delta(v)| < \min\left\{\frac{\Delta^2}{4}, \frac{n}{4}\right\}\right) \leq \frac{c_1}{\Delta^2}.$$

Proof. First of all, observe that for $\Delta \leq 2$ the statement is trivial since in that case we have $c_1/\Delta^2 \geq 1$. Therefore, from now on assume w.l.o.g. that $\Delta > 2$. Let $s_\Delta := \min\{\Delta^2/4, n/4\}$. Using Lemma 11 with $k = s_\Delta$ we obtain

$$\mathbb{P}\left(|B_\Delta(v)| < s_\Delta\right) \leq \frac{\sqrt{s_\Delta - 1}}{\Delta} \cdot \exp\left(-2(\sqrt{s_\Delta}-1)\left(\frac{\Delta}{\sqrt{s_\Delta - 1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{s_\Delta - 1}}\right)\right)\right).$$

So, it remains to show that there exists a constant c_1 such that for any $\Delta > 2$ we have

$$\Delta\sqrt{s_\Delta - 1} \cdot \exp\left(-2(\sqrt{s_\Delta}-1)\left(\frac{\Delta}{\sqrt{s_\Delta - 1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{s_\Delta - 1}}\right)\right)\right) \leq c_1.$$

The tedious computations needed to show that this is true can be found in Appendix A. ◀

Clustering

The following theorem shows that we can partition the vertices of sparse random shortest path metrics into a suitably small number of clusters with a given maximum diameter. Its proof follows closely the ideas of Bringmann et al. [6], albeit with a different value of s_Δ.

▶ **Theorem 13.** *Let G be a finite square grid graph on $n = N^2$ vertices, consider a (sparse) random shortest path metric generated using this graph, and let $\Delta > 0$. There exists a partition of vertices into clusters, each of diameter at most 4Δ, such that the expected number of clusters needed is bounded from above by $O(1 + n/\Delta^2)$, where constant of the O-term is uniform with respect to Δ.*

Proof. Let n be sufficiently large ($n \geq 9$ suffices) and let $s_\Delta := \min\{\Delta^2/4, n/4\}$, as in Corollary 12. We call vertex v Δ-dense if $|B_\Delta(v)| \geq s_\Delta$ and Δ-sparse otherwise. Using Corollary 12 we can bound the expected number of Δ-sparse vertices by $O(n/\Delta^2)$. We put each Δ-sparse vertex in its own cluster (of size 1), which has diameter $0 \leq 4\Delta$.

Now, only the Δ-dense vertices remain. We cluster them according to the following process. Consider an auxiliary graph H whose vertices are the Δ-dense vertices and where two vertices u, v are connected by an edge if and only if $B_\Delta(u) \cap B_\Delta(v) \neq \varnothing$. Consider an arbitrary maximal independent set S in H, and observe that $|S| \leq n/s_\Delta$ by construction of H. We create the initial clusters $C_1, \dots, C_{|S|}$, each of which equals $B_\Delta(v)$ for some vertex $v \in S$. These initial clusters have diameter at most 2Δ.

Next, consider an arbitrary Δ-dense vertex v that is not yet part of any cluster. By the maximality of S, we know that there must exist a vertex $u \in S$ such that $A := B_\Delta(u) \cap B_\Delta(v) \neq \varnothing$. Let $x \in A$ be arbitrarily chosen, and observe that $d(v, u) \leq d(v, x) + d(x, u) \leq \Delta + \Delta = 2\Delta$. We add v to the initial cluster corresponding to u, and repeat this step until all Δ-dense vertices have been added to some initial cluster. By construction, the diameter of all these clusters is now at most 4Δ: consider two arbitrary vertices w, y in a cluster that initially corresponded to $u \in S$; then we have $d(w, y) \leq d(w, u) + d(u, y) \leq 2\Delta + 2\Delta = 4\Delta$.

So, now we have in expectation at most $O(n/\Delta^2)$ clusters containing one (Δ-sparse) vertex each, and at most $n/s_\Delta = O(1 + n/\Delta^2)$ clusters containing at least s_Δ (Δ-dense) vertices each, all with diameter at most 4Δ. The result follows. ◀

A Tail Bound for $\Delta_{\max}$

Recall that $\Delta_{\max} = \max_{u,v} d(u, v)$ is the diameter of the random metric. The following lemma shows that $\Delta_{\max} \leq O(\sqrt{n})$ with high probability. Due to space constraints, its proof can be found in Appendix B.

▶ **Lemma 14.** *Let $x \geq 9\sqrt{n}$. Then we have $\mathbb{P}(\Delta_{\max} \geq x) \leq ne^{-x}$.*

4 Analyses of Greedy-like Heuristics for Matching and TSP

In this section, we show that three greedy-like heuristics (greedy for minimum-distance perfect matching, and nearest neighbor and insertion for TSP) achieve a constant expected approximation ratio on sparse random shortest path metrics generated from a finite square grid graph. The three proofs are very alike, and the ideas behind them are built upon ideas by Bringmann et al. [6]: we divide the steps of the greedy-like heuristics into bins, depending on the value which they add to the total distance of our matching or TSP tour. Using the clustering (Theorem 13) we bound the total contribution of these bins by $O(n)$, and using our observation regarding sums of lightest edge weights (Lemmas 6 and 7) we show that the optimal matching or TSP tour has a distance of $\Omega(n)$ with sufficiently high probability.

Greedy Heuristic for Minimum-Distance Perfect Matching

The first problem that we consider is the minimum-distance perfect matching problem. Even though solving the minimum-distance perfect matching problem to optimality is not very difficult (it can be done in $O(n^3)$ time), in practice this is often too slow, especially if the number of vertices is large. Therefore, people often rely on (simple) heuristics to solve this problem in practical situations. The greedy heuristic is arguably the simplest one among these heuristics. It starts with an empty matching and iteratively adds a pair of currently unmatched vertices (an "edge") to the matching such that the distance between them is minimal. Let GR denote the total distance of the matching computed by the greedy heuristic, and let MM denote the total distance of an optimal matching.

It is known that the worst-case approximation ratio for this heuristic on metric instances is $O(n^{\log_2(3/2)})$ [19]. Moreover, for random Euclidean instances, the greedy heuristic has an approximation ratio of $O(1)$ with high probability [2], and for random shortest path metrics generated from complete graphs or Erdős–Rényi random graphs the expected approximation ratio of the greedy heuristic is $O(1)$ as well [6, 18]. We show that a similar result holds for sparse random shortest path metrics generated from a finite square grid graph.

▶ **Theorem 15.** $\mathbb{E}[\mathsf{GR}] = O(n)$.

Proof. We put "edges" that are being added to the greedy matching into bins according to their distance: bin i receives all "edges" $\{u, v\}$ with $d(u, v) \in \big(4(i-1), 4i\big]$. Let X_i denote the number of "edges" that end up in bin i and set $Y_i := \sum_{k=i}^{\infty} X_k$, i.e., Y_i is the number of "edges" in the greedy matching with distance at least $4(i-1)$. Observe that $Y_1 = n/2$. For $i > 1$, by Theorem 13, we can partition the vertices in an expected number of $O(1 + n/(i-1)^2)$ clusters (where the constant of the O-term is uniform with respect to i), each of diameter at most $4(i-1)$. Just before the greedy heuristic adds for the first time an "edge" of distance more than $4(i-1)$, it must be the case that each of these clusters contains at most one unmatched vertex (otherwise the greedy heuristic would have chosen an "edge" between two vertices in the same cluster). Therefore, we can conclude that $\mathbb{E}[Y_i] \le O(1 + n/(i-1)^2)$ for $i > 1$. On the other hand, for $4(i-1) \ge 9\sqrt{n}$, it follows from Lemma 14 that $\mathbb{E}[Y_i] \le n \cdot \mathbb{P}(\Delta_{\max} \ge 4(i-1)) \le n^2 e^{-4(i-1)}$.

Now we sum over all bins, bound the length of each "edge" in bin i by $4i$, and subsequently use Fubini's theorem and the derived bounds on $\mathbb{E}[Y_i]$. This yields

$$\begin{aligned}\mathbb{E}[\mathsf{GR}] &\le \sum_{i=1}^{\infty} 4i \cdot \mathbb{E}[X_i] = \sum_{i=1}^{\infty} 4 \cdot \mathbb{E}[Y_i] = 2n + \sum_{i=2}^{3\sqrt{n}} 4 \cdot \mathbb{E}[Y_i] + \sum_{i=3\sqrt{n}}^{\infty} 4 \cdot \mathbb{E}[Y_i] \\ &\le 2n + \sum_{i=2}^{3\sqrt{n}} O\left(1 + \frac{n}{(i-1)^2}\right) + \sum_{i=3\sqrt{n}}^{\infty} 4n^2 e^{-4(i-1)} = O(n) + O(n) + o(1) = O(n),\end{aligned}$$

which finishes the proof. ◀

▶ **Theorem 16.** *For random shortest path metrics generated from a finite grid graph we have* $\mathbb{E}\left[\frac{\mathsf{GR}}{\mathsf{MM}}\right] = O(1)$.

Proof. Let $c > 0$ be a sufficiently small constant. Then the approximation ratio of the greedy heuristic on random shortest path metrics generated from a finite grid graph is

$$\mathbb{E}\left[\frac{\mathsf{GR}}{\mathsf{MM}}\right] \le \mathbb{E}\left[\frac{\mathsf{GR}}{cn}\right] + \mathbb{P}\left(\mathsf{MM} < cn\right) \cdot O\left(n^{\log_2(3/2)}\right),$$

since the worst-case approximation ratio of the greedy heuristic on metric instances is $O(n^{\log_2(3/2)})$ [19]. By Theorem 15 the first term is $O(1)$. Combining Lemmas 6 and 7, the second term can be bounded from above by $\exp(n(1+\frac{1}{2}\ln(c\cdot\Theta(1))))\cdot O(n^{\log_2(3/2)}) = o(1)$ since c is sufficiently small. ◀

Nearest Neighbor Heuristic for TSP

One of the most intuitive heuristics for the TSP is the nearest neighbor heuristic. This greedy-like heuristic starts with an arbitrary vertex as its current vertex and iteratively builds a TSP tour by traveling from its current vertex to the closest unvisited vertex and adding the corresponding "edge" to the tour (and closing the tour by going back to its first vertex after all vertices have been visited). Let NN denote the total distance of the TSP tour computed by the nearest neighbor heuristic, and let TSP denote the total distance of an optimal TSP tour.

It is known that the worst-case approximation ratio for this heuristic on metric instances is $O(\ln(n))$ [21]. Moreover, for random Euclidean instances, the nearest neighbor heuristic has an approximation ratio of $O(1)$ with high probability [3], and for random shortest path metrics generated from complete graphs or Erdős–Rényi random graphs the expected approximation ratio of the nearest neighbor heuristic is $O(1)$ as well [6, 18]. We show that a similar result holds for sparse random shortest path metrics generated from a finite square grid graph.

▶ **Theorem 17.** $\mathbb{E}[\mathsf{NN}] = O(n)$.

Proof. We put "edges" that are being added to the nearest neighbor TSP tour into bins according to their distance: bin i receives all "edges" $\{u,v\}$ with $d(u,v)\in\big(4(i-1),4i\big]$. Let X_i and Y_i be defined as in the proof of Theorem 15. Now we have $Y_1 = n$. For $i>1$, by Theorem 13, we can partition the vertices in an expected number of $O(1+n/(i-1)^2)$ clusters (where the constant of the O-term is uniform with respect to i), each of diameter at most $4(i-1)$. Every time the nearest neighbor heuristic adds an "edge" of distance more than $4(i-1)$, this must be an "edge" from a vertex in some cluster C_k to a vertex in another cluster C_ℓ, and the tour must have already visited all other vertices in C_k (otherwise the nearest neighbor heuristic would have chosen an "edge" to an unvisited vertex in C_k). Therefore, we can conclude that $\mathbb{E}[Y_i]\le O(1+n/(i-1)^2)$ for $i>1$. On the other hand, for $4(i-1)\ge 9\sqrt{n}$, it follows from Lemma 14 that $\mathbb{E}[Y_i]\le n\cdot\mathbb{P}(\Delta_{\max}\ge 4(i-1))\le n^2e^{-4(i-1)}$.

Note that we have derived exactly the same bounds as in the proof of Theorem 15. So, using the same calculations as in that proof, it follows now that $\mathbb{E}[\mathsf{NN}] = O(n)$. ◀

▶ **Theorem 18.** *For random shortest path metrics generated from a finite grid graph we have* $\mathbb{E}\left[\frac{\mathsf{NN}}{\mathsf{TSP}}\right] = O(1)$.

The proof of this theorem is similar to that of Theorem 16, with the worst-case approximation ratio of the nearest neighbor heuristic on metric instances being $O(\ln(n))$ [21].

Insertion Heuristics for TSP

Another group of greedy-like heuristics for the TSP are the insertion heuristics. An insertion heuristic starts with an initial optimal tour on a few vertices that are selected according to some predefined rule R, and iteratively chooses (according to the same rule R) a vertex that is not in the tour yet and inserts this vertex in the current tour such that the total distance of the tour increases the least. An example of such a rule R would be to start with an initial (optimal) tour on three arbitrary vertices, and then use farthest insertion, i.e., at each step insert the vertex whose minimal distance to a vertex already in the tour is maximal.

Let IN_R denote the total distance of the TSP tour computed by the insertion heuristic using rule R, and let TSP denote the total distance of an optimal TSP tour. It is known that the worst-case approximation ratio for this heuristic for any rule R on metric instances is $O(\ln(n))$ [21]. Moreover, for random shortest path metrics generated from complete graphs or Erdős–Rényi random graphs the expected approximation ratio of the nearest neighbor heuristic is $O(1)$ for any rule R [6, 18]. We show that a similar result holds for sparse random shortest path metrics generated from a finite square grid graph.

▶ **Theorem 19.** $\mathbb{E}[\mathsf{IN}_R] = O(n)$.

Proof. We put the steps of the insertion heuristic into bins according to the distance they add to the tour: bin i receives all steps with a contribution in the range $\big(8(i-1), 8i\big]$. Let X_i and Y_i be defined as in the proof of Theorem 15. Again we have $Y_1 = n$. For $i > 1$, by Theorem 13, we can partition the vertices in an expected number of $O(1+n/(i-1)^2)$ clusters (where the constant of the O-term is uniform with respect to i), each of diameter at most $4(i-1)$. Every time the contribution of a step of the insertion heuristic is more than $8(i-1)$, this step must add a vertex to the tour that is part of a cluster C_k of which no other vertex is in the tour yet (otherwise the contribution of this step would have been less than $8(i-1)$). Therefore, we can conclude that $\mathbb{E}[Y_i] \le O(1+n/(i-1)^2)$ for $i > 1$. On the other hand, for $8(i-1) \ge 9\sqrt{n}$, it follows from Lemma 14 that $\mathbb{E}[Y_i] \le 2n \cdot \mathbb{P}(\Delta_{\max} \ge 8(i-1)) \le 2n^2 e^{-8(i-1)}$.

Using the same method as in the proof of Theorem 15 (i.e., summing over all bins, bounding the contribution of each step in bin i by $8i$ and using Fubini's theorem and the derived bounds on $\mathbb{E}[Y_i]$), and adding the expected contribution $\mathbb{E}[T_R]$ of the initial tour, yields

$$\begin{aligned}
\mathbb{E}[\mathsf{IN}_R] &\le \mathbb{E}[T_R] + \sum_{i=1}^{\infty} 8i \cdot \mathbb{E}[X_i] = \mathbb{E}[T_R] + \sum_{i=1}^{\infty} 8 \cdot \mathbb{E}[Y_i] \\
&= \mathbb{E}[T_R] + 8n + \sum_{i=2}^{2\sqrt{n}} 8 \cdot \mathbb{E}[Y_i] + \sum_{i=2\sqrt{n}}^{\infty} 8 \cdot \mathbb{E}[Y_i] \\
&\le O(n) + 8n + \sum_{i=2}^{2\sqrt{n}} O\left(1 + \frac{n}{(i-1)^2}\right) + \sum_{i=2\sqrt{n}}^{\infty} 16n^2 e^{-8(i-1)} = O(n),
\end{aligned}$$

where we used Theorem 17 to bound the expected contribution of the initial tour by $\mathbb{E}[T_R] \le \mathbb{E}[\mathsf{TSP}] \le \mathbb{E}[\mathsf{NN}] = O(n)$. Observe that this proof is independent of the choice of rule R. ◀

▶ **Theorem 20.** *For random shortest path metrics generated from a finite grid graph we have* $\mathbb{E}\left[\frac{\mathsf{IN}_R}{\mathsf{TSP}}\right] = O(1)$.

The proof of this theorem is similar to that of Theorem 16, with the worst-case approximation ratio of the insertion heuristic on metric instances being $O(\ln(n))$ [21].

5 Analysis of 2-opt for TSP

In this section, we consider the probably most famous local search heuristic for the TSP, the 2-opt heuristic, and show that it achieves a constant expected approximation ratio as well. Since we do not make use of any of the lemmas that have been tailored to random shortest path metrics generated from finite square grid graphs, the results in this section hold for random shortest path metrics generated from any sparse graph.

The 2-opt heuristic starts with an arbitrary initial solution and iteratively improves this solution by applying so-called 2-exchanges until no improvement is possible anymore. In a 2-exchange, two "edges" $\{u_1, v_1\}$ and $\{u_2, v_2\}$ that are visited in this order in the current solution are removed from it and replaced by the two "edges" $\{u_1, u_2\}$ and $\{v_1, v_2\}$ to obtain a new solution. The improvement of this 2-exchange is $\delta = d(u_1, v_1)+d(u_2, v_2)-d(u_1, u_2)-d(v_1, v_2)$. A solution is called 2-optimal if $\delta \leq 0$ for all possible 2-exchanges.

The actual performance of the 2-opt heuristic strongly depends on the choice of the initial solution and the sequence of improvements. In this paper we look at the worst possible outcome of the 2-opt heuristic, as others have been doing before (see e.g. [7, 9]), since this decouples the actual heuristic from the initialization and therefore keeps the analysis tractable. Let WLO denote the total distance of the worst 2-optimal TSP tour, and let TSP denote the total distance of an optimal TSP tour.

It is known that the worst-case approximation ratio for this heuristic on metric instances is $O(\sqrt{n})$ [7]. Moreover, for Euclidean instances, the 2-opt heuristic has an expected approximation ratio of $O(1)$ [7]. For random shortest path metrics on complete graphs, there is a trivial upper bound of $O(\ln(n))$ for the expected approximation ratio of the 2-opt heuristic, but it is an open problem whether this can be improved or not [6]. We show that for random shortest path metrics generated from sparse graphs, the expected approximation ratio of the 2-opt heuristic is $O(1)$.

The crucial observation that enables us to show this result is the fact that for any 2-optimal solution for the TSP it holds that each edge $e \in E$ can appear at most twice in the disjoint union of all shortest paths that correspond to this solution. In other words, the total distance of any 2-optimal solution can be bounded by twice the sum of all edge weights in G. The following lemma and theorems formalize this observation and its consequences.

▶ **Lemma 21.** *Consider a 2-optimal solution for the TSP. For each $i, j \in V$, let P_{ij} denote the set of all (directed) edges in the shortest i, j-path. Moreover, let $x_{ij} = 1$ if the solution travels directly from vertex i to vertex j, and $x_{ij} := 0$ otherwise. Then, for any $i, j, k, l \in V$ with $x_{ij} = x_{kl} = 1$ we have either $P_{ij} \cap P_{kl} = \varnothing$ or $(i, j) = (k, l)$.*

Proof. Let $i, j, k, l \in V$ such that $x_{ij} = x_{kl} = 1$, and suppose that $(i, j) \neq (k, l)$. Set $A := \{i, j, k, l\}$ and observe that $|A|$ equals either 3 or 4. ($|A| = 2$ would imply $(i, j) = (k, l)$.)

First, suppose that $|A| = 4$. Suppose, by way of contradiction, that $P_{ij} \cap P_{kl} \neq \varnothing$. Take $e = (s, t) \in P_{ij} \cap P_{kl}$. Then $d(i, j) = d(i, s)+w(e)+d(t, j)$ and $d(k, l) = d(k, s)+w(e)+d(t, l)$. Moreover, using the triangle inequality, we can see that $d(i, k) \leq d(i, s) + d(s, k)$ and $d(j, l) \leq d(j, t) + d(t, l)$. Let $\delta = \delta(i, j, k, l)$ denote the improvement of the 2-exchange where $\{i, j\}$ and $\{k, l\}$ are replaced by $\{i, k\}$ and $\{j, l\}$, and note that $\delta \leq 0$ since we are considering a 2-optimal solution for the TSP. It follows that

$$\begin{aligned}
0 \geq \delta &= d(i, j) + d(k, l) - d(i, k) - d(j, l) \\
&\geq d(i, s) + w(e) + d(t, j) + d(k, s) + w(e) + d(t, l) - d(i, s) - d(s, k) - d(j, t) - d(t, l) \\
&= 2w(e) > 0,
\end{aligned}$$

which is clearly a contradiction. Therefore we must have $P_{ij} \cap P_{kl} = \varnothing$ in this case.

Now, suppose that $|A| = 3$. Since the x variables describe a solution to the TSP, this implies that either $j = k$ or $i = l$. These cases are analogously, so w.l.o.g. we assume that $j = k$. The proof that $P_{ij} \cap P_{kl} = \varnothing$ in this case is similar to the proof for $|A| = 4$, with the exception that here we have $\delta = d(i, j) + d(j, l) - d(i, j) - d(j, l) = 0$ (instead of $\delta \leq 0$). The result follows. ◀

▶ **Theorem 22.** $\mathbb{E}[\mathsf{WLO}] = O(n)$.

Proof. For each $i, j \in V$, let P_{ij} denote the set of all (directed) edges in the shortest i,j-path. Moreover, let $x_{ij} = 1$ if WLO travels directly from vertex i to vertex j, and $x_{ij} = 0$ otherwise.

From Lemma 21 we know that each edge $e \in E$ can appear at most twice in the disjoint union of all shortest i,j-paths that form a 2-optimal tour (at most once per direction). This yields

$$\mathsf{WLO} = \sum_{i,j \in V} d(i,j) x_{ij} = \sum_{\substack{i,j \in V \\ x_{ij}=1}} \sum_{e \in P_{ij}} w(e) \le \sum_{e \in E} 2w(e) = 2S_{|E|},$$

where S_m denotes the sum of the m lightest edge weights in G as before. Combining this with Corollary 5, it follows that

$$\mathbb{E}[\mathsf{WLO}] \le \mathbb{E}\left[2S_{|E|}\right] = O\left(\frac{|E|^2}{n}\right) = O(n),$$

where the last equality follows by recalling that $|E| = \Theta(n)$ for sparse graphs. ◀

▶ **Theorem 23.** *For random shortest path metrics generated from a sparse graph we have* $\mathbb{E}\left[\frac{\mathsf{WLO}}{\mathsf{TSP}}\right] = O(1)$.

The proof of this theorem is similar to that of Theorem 16, with the worst-case approximation ratio of the 2-opt heuristic on metric instances being $O(\sqrt{n})$ [7].

6 Concluding Remarks

We have analyzed simple heuristics for matching and TSP on random shortest path metrics generated from sparse graphs, since we believe that these models yield more realistic metric spaces than random shortest path metrics generated from dense or even complete graphs. However, for the greedy-like heuristics we had to restrict ourselves to (finite square) grid graphs. It is possible to adapt our proofs for all classes of sparse graphs that have sufficiently fast growing cut sizes $|\delta(U)|$ (as long as $|U|$ is not too large). It seems to be sufficient to have $|\delta(U)| \ge \Omega(|U|^\varepsilon)$ if $|U| \le c'n$ for some constants $\varepsilon, c' \in (0,1)$. Sparse graphs that have this property include d-dimensional grid graphs and other lattice graphs. We raise the question whether it is possible to extend our findings for these heuristics to arbitrary sparse graphs.

On the other hand, especially if we consider random shortest path metrics generated from grid graphs, in our view the model could be improved by using only a (possibly random) subset of the vertices of G for defining the random metric space, i.e., restricting the distance function d of the metric to some sub-domain $V' \times V'$, where $V' \subset V$. It would be interesting to see whether this model could be analyzed as well.

Finally, in our analysis of the 2-opt local search heuristic, we had to decouple the actual heuristic from the initialization in order to make the analysis tractable. We leave it as an open problem to prove rigorous results about hybrid heuristics that consist of an initialization and a local search algorithm.

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A Computations for the Proof of Corollary 12

In this appendix we show that there exists a constant c_1 such that for any $\Delta > 2$ we have

$$\Delta\sqrt{s_\Delta - 1}\cdot\exp\left(-2(\sqrt{s_\Delta}-1)\left(\frac{\Delta}{\sqrt{s_\Delta-1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{s_\Delta-1}}\right)\right)\right) \leq c_1,$$

where $s_\Delta := \min\{\Delta^2/4, n/4\}$ and $n \geq 9$. We consider two cases: $\Delta^2 \leq n$ and $\Delta^2 \geq n$.

For the first case, suppose that $\Delta^2 \leq n$. Then we have $s_\Delta = \Delta^2/4$, and we need to show that

$$f(\Delta) := \Delta\sqrt{\Delta^2/4 - 1}\cdot\exp\left(-(\Delta-2)\left(\frac{\Delta}{\sqrt{\Delta^2/4-1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{\Delta^2/4-1}}\right)\right)\right) \leq c_1.$$

Now observe that $\lambda - 1 - \ln(\lambda)$ is an increasing function of λ for $\lambda \geq 1$. Combining this with the observation that $\sqrt{\Delta^2/4-1} \leq \sqrt{\Delta^2/4} = \Delta/2$ (for any $\Delta \geq 2$), it follows now that

$$f(\Delta) \leq \tfrac{1}{2}\Delta^2 e^{-(\Delta-2)(1-\ln(2))}.$$

So, $f(\Delta)$ is upper bounded by a function $g(\Delta)$ of the form $g(\Delta) = c_2\Delta^2 e^{-c_3\Delta}$ for some constants $c_2, c_3 \geq 0$. It is well-established that such a function has a finite global maximum (which can be shown to be equal to $\frac{1}{4}c_2c_3^2e^{-c_3^2/2}$). Therefore, we can conclude that in this case there exists a constant c_1 such that $f(\Delta) \leq c_1$ for all $\Delta > 2$.

For the second case, suppose that $\Delta^2 \geq n$. Then we have $s_\Delta = n/4$, and we need to show that we have

$$h(\Delta, n) := \Delta\sqrt{n/4-1}\cdot\exp\left(-(\sqrt{n}-2)\left(\frac{\Delta}{\sqrt{n/4-1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{n/4-1}}\right)\right)\right) \leq c_1,$$

for all pairs (Δ, n) satisfying $\Delta^2 \geq n \geq 9$. The first step of the proof is to show that $h(\Delta, n) \leq h(\sqrt{n}, n)$ for all $\Delta \geq \sqrt{n}$. To do so, we compute the partial derivative of $h(\Delta, n)$ with respect to Δ, and show that it is non-positive for all $\Delta \geq \sqrt{n}$. The partial derivative equals

$$\frac{\partial h(\Delta,n)}{\partial\Delta} = \left(\sqrt{n/4-1} - (\sqrt{n}-2)(\Delta - \sqrt{n/4-1})\right) \cdot\exp\left(-(\sqrt{n}-2)\left(\frac{\Delta}{\sqrt{n/4-1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{n/4-1}}\right)\right)\right).$$

Now observe that for all $n \geq 9$ we have

$$\sqrt{n/4-1} \cdot \frac{\sqrt{n}-1}{\sqrt{n}-2} \leq \sqrt{n/4} \cdot 2 = \sqrt{n} \leq \Delta.$$

This inequality can be rewritten into $\sqrt{n/4-1} - (\sqrt{n}-2)(\Delta - \sqrt{n/4-1}) \leq 0$, which (together with the fact that $e^x > 0$ for all $x \in \mathbb{R}$) shows that the partial derivative of $h(\Delta, n)$ with respect to Δ is indeed non-positive for all $\Delta \geq \sqrt{n}$. So, we may now conclude that $h(\Delta, n) \leq h(\sqrt{n}, n)$ for all $\Delta \geq \sqrt{n}$.
Next, notice that $h(\sqrt{n}, n) = f(\sqrt{n})$. In the first case we have already shown that there exists a constant c_1 such that $f(\Delta) \leq c_1$ for all $\Delta > 2$. So, it follows immediately that $h(\Delta, n) \leq h(\sqrt{n}, n) = f(\sqrt{n}) \leq c_1$ for all pairs (Δ, n) satisfying $\Delta^2 \geq n \geq 9$.

Combining both cases, we can now see that indeed there exists a constant c_1 such that for any $\Delta > 2$ we have

$$\Delta\sqrt{s_\Delta - 1} \cdot \exp\left(-2(\sqrt{s_\Delta}-1)\left(\frac{\Delta}{\sqrt{s_\Delta - 1}} - 1 - \ln\left(\frac{\Delta}{\sqrt{s_\Delta - 1}}\right)\right)\right) \leq c_1,$$

where $s_\Delta := \min\{\Delta^2/4, n/4\}$ and $n \geq 9$.

▶ Remark. Numerical computations show that $c_1 \geq 4.0647$ is sufficient for this result to hold.

B Proof of Lemma 14

▶ **Lemma 14.** *Let $x \geq 9\sqrt{n}$. Then we have $\mathbb{P}(\Delta_{\max} \geq x) \leq ne^{-x}$.*

Proof. Fix an arbitrary $v \in V$ and recall that we assume n to be even (the proof for odd n is similar, but requires some more care with the bounds of the summations). We first show that $\mathbb{P}(\tau_n(v) \geq x) \leq e^{-x}$. Using a similar argument as in the proof of Corollary 9, we can derive from Lemma 8 that

$$\tau_n(v) \precsim \sum_{i=1}^{\frac{1}{4}n-1} \mathrm{Exp}(2\sqrt{i}) + \sum_{i=\frac{1}{4}n}^{\frac{3}{4}n} \mathrm{Exp}(\sqrt{n}) + \sum_{i=\frac{3}{4}n+1}^{n-1} \mathrm{Exp}(2\sqrt{n-i}).$$

From this, we can see that

$$\mathbb{P}\left(\tau_n(v) \geq x\right) \leq \mathbb{P}\left(\sum_{i=1}^{\frac{1}{4}n-1} \mathrm{Exp}(2\sqrt{i}) + \sum_{i=\frac{1}{4}n}^{\frac{3}{4}n} \mathrm{Exp}(\sqrt{n}) + \sum_{i=\frac{3}{4}n+1}^{n-1} \mathrm{Exp}(2\sqrt{n-i}) \geq x\right).$$

In order to bound this probability, we once more use Lemma 1(i). For this purpose, set

$$\mu := \mathbb{E}\left[\sum_{i=1}^{\frac{1}{4}n-1} \mathrm{Exp}(2\sqrt{i}) + \sum_{i=\frac{1}{4}n}^{\frac{3}{4}n} \mathrm{Exp}(\sqrt{n}) + \sum_{i=\frac{3}{4}n+1}^{n-1} \mathrm{Exp}(2\sqrt{n-i})\right] = \frac{n+2}{2\sqrt{n}} + \sum_{i=1}^{\frac{1}{4}n-1} \frac{1}{\sqrt{i}},$$

and $\lambda := x/\mu$, and observe that $\mu \leq \frac{1}{2}\sqrt{n} + \sqrt{n-4} + 1/\sqrt{n} \leq \frac{3}{2}\sqrt{n}$. Together with $x \geq 9\sqrt{n}$ this implies $\lambda \geq 6$. Lemma 1(i) now yields

$$\mathbb{P}\left(\tau_n(v) \geq x\right) \leq \lambda^{-1}e^{-2\mu(\lambda-1-\ln(\lambda))} \leq e^{-2\mu(\lambda/2)} = e^{-\lambda\mu} = e^{-x},$$

where we used $\lambda - 1 - \ln(\lambda) \geq \lambda/2$ (which holds for all $\lambda \geq 5.36$) for the second inequality. The final results follows from observing that $\Delta_{\max} = \max_v \tau_n(v)$ and applying the appropriate union bound. ◀

Greedy Maximal Independent Sets via Local Limits

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Abstract

The random greedy algorithm for finding a maximal independent set in a graph has been studied extensively in various settings in combinatorics, probability, computer science – and even in chemistry. The algorithm builds a maximal independent set by inspecting the vertices of the graph one at a time according to a random order, adding the current vertex to the independent set if it is not connected to any previously added vertex by an edge.

In this paper we present a natural and general framework for calculating the asymptotics of the proportion of the yielded independent set for sequences of (possibly random) graphs, involving a useful notion of local convergence. We use this framework both to give short and simple proofs for results on previously studied families of graphs, such as paths and binomial random graphs, and to study new ones, such as random trees.

We conclude our work by analysing the random greedy algorithm more closely when the base graph is a tree. We show that in expectation, the cardinality of a random greedy independent set in the path is no larger than that in any other tree of the same order.

2012 ACM Subject Classification Mathematics of computing → Graph algorithms; Mathematics of computing → Random graphs; Mathematics of computing → Probabilistic algorithms

Keywords and phrases Greedy maximal independent set, random graph, local limit

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.20

Related Version A full version of the paper is available at `https://arxiv.org/abs/1907.07216`.

Funding *Michael Krivelevich*: Partially supported by USA–Israel BSF grants 2014361 and 2018267, and by ISF grant 1261/17.
Tamás Mészáros: Research supported by the Dahlem Research School and by the Berlin Mathematics Research Center Math+.
Peleg Michaeli: This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement number 676970, RANDGEOM).

Acknowledgements The authors wish to thank the organisers of the Joint FUB–TAU Workshop on Graph and Hypergraph Colouring, hosted by the Freie Universität Berlin in 2018, and Michal Amir, Shagnik Das, Lior Gishboliner, Matan Harel, Frank Mousset, Matan Shalev and Yinon Spinka for useful discussions and ideas.

1 Introduction

Algorithmic problems related to finding or approximating the independence number of a graph, or to producing large independent sets, have long been in the focus of the computer science community. Computing the size of a *maximum* independent set is known to be NP-complete [30] and the groundbreaking work [16] on the difficulty of approximating it even made its way to The New York Times. A natural way to try to efficiently produce a large independent set in an input graph G is to output a *maximal* independent set (MIS) in G, where a vertex subset $I \subseteq V(G)$ is a MIS in G if I is maximal by inclusion. While in principle a badly chosen MIS can be very small (like, say, the star center in a star), one might hope that quite a few of the maximal independent sets will have size comparable in some sense to the independence number of G.

In this paper, we study the *random* greedy algorithm for producing a maximal independent set, which is defined as follows. Consider an input graph G on n vertices. The algorithm first orders the vertices of G uniformly at random, and then builds an independent set $\mathbf{I}(G)$ by considering each of the vertices v one by one in order, adding v to $\mathbf{I}(G)$ if the resulting set does not span any edge. Observe that the set $\mathbf{I}(G)$ is in fact the set of vertices coloured in the first colour in a random greedy proper colouring of G. A basic quantity to study, which turns out to have numerous applications, is the proportion of the yielded independent set (which we call the **greedy independence ratio**). In particular, it is of interest to study the asymptotic behaviour of this quantity for natural graph sequences.

Due to its simplicity, this greedy algorithm has been studied extensively by various authors in different fields, ranging from combinatorics [48], probability [42] and computer science [18] to chemistry [20]. As early as 1931 this model was studied by chemists under the name *random sequential adsorption* (RSA), focusing mostly on d-dimensional grids. The 1-dimensional case was solved by Flory [20] (see also [38]), who showed that the expected greedy independence ratio tends to $\zeta_2 = (1 - e^{-2})/2$ as the path length tends to infinity.

A continuous analogue, where "cars" of unit length "park" at random free locations on the interval $[0, X]$, was introduced (and solved) by Rényi [43], under the name *car-parking process*. The limiting density, as X tends to infinity, is therefore called **Rényi's parking constant**, and ζ_2 may be considered as its discrete counterpart (see, e.g., [17]). Following this terminology, the final state of the car-parking process is often called the *jamming limit* of the graph, and the density of this state is called the *jamming constant*. For dimension 2, Palásti [39] conjectured, in the continuous case (where unit square "cars" park in a larger square), that the limiting density is Rényi's parking constant squared. This conjecture may be carried over to the discrete case, but to the best of our knowledge, in both cases it remains open. For further details see [17] (see also [15] for an extensive survey on RSA models).

In combinatorics, the greedy algorithm for finding a maximal independent set was analysed in order to give a lower bound on the (usually asymptotic) typical independence number of (random) graphs[1]. The asymptotic greedy independence ratio of binomial random graphs with linear edge density was studied by McDiarmid [35] (but see also [25, 9]). The asymptotic greedy independence ratio of random regular graphs was studied by Wormald [48], who used the so-called *differential equation method* (see [49] for a comprehensive survey; see also [47] for a short proof of Wormald's result). His result was further extended in [33] for any regular graph sequence with growing girth (see also [29, 28] for similar extensions for more sophisticated algorithms). Recently, the case of uniform random graphs with given degree sequences was studied (independently) in [5] and [11].

[1] In this regard, the greedy algorithm has long been superseded by more sophisticated algorithms; these algorithms often lack, however, the local properties of the greedy algorithm.

In a more general setting, where we run the random greedy algorithm on a *hypergraph*, the model recovers in particular the *triangle-free process* (or, more generally, the *H-free process*). In this process, which was first introduced in [14], we begin with the empty graph, and at each step add a random edge as long as it does not create a copy of a triangle (or a copy of H). To recover this process we take the hypergraph whose vertices are the edges of the complete graph, and whose hyperedges are the triples of edges that span a triangle (or k-sets of edges that form a copy of H, if H has k edges). Bohman's key result [7] is that for this hypergraph, $|\mathbf{I}|$ is asymptotically almost surely $\Theta(n^{3/2}\sqrt{\ln n})$, where n is the number of vertices. The exact asymptotics was later found by Bohman and Keevash [8] and by Fiz Pontiveros, Griffiths and Morris [19]. Similar results were obtained for the complete graph on 4 vertices by Warnke [46] and for cycles independently by Picollelli [41] and by Warnke [45]. For a discussion about the general setting, see [4].

Consider the following alternative but equivalent definition of the model. Assign an independent uniform *label* from $[0, 1]$ to each vertex of the graph, and consider it as the *arrival time* of a particle at that vertex. All vertices are initially vacant, and a vertex becomes occupied at the time denoted by its label if and only if all of its neighbours are still vacant at that time. Clearly, we do not need to worry that two particles will arrive at the same time. The set of occupied vertices at time 1 is exactly the greedy MIS. The advantage of this formulation of the model is that under mild assumptions, it can be defined on an infinite graph. We may think of the resulting MIS as a *factor of iid* (**fiid**)[2], meaning, informally, that there exists a local rule which is unaware of the "identity" of a given vertex, that determines whether that vertex is occupied. It was conjectured (formally by Hatami, Lovász and Szegedy [26]) that, using a proper rule, **fiid** can produce an asymptotically maximum independent set in random regular graphs. However, this was disproved recently by Gamarnik and Sudan [23]. In fact, they showed that this kind of local algorithms has a uniformly limited power for sufficiently large degree, and later Rahman and Virág [42] showed that the density of **fiid** independent sets in regular trees and in Poisson Galton–Watson trees, with large average degree, is asymptotically at most half-optimal, concluding (after projecting to random regular graphs or to binomial random graphs) that local algorithms cannot achieve better.

However, on other families of graphs, local algorithms may clearly do better than that. A trivial example is the set of stars, where the greedy algorithm typically performs perfectly. A less trivial example is that of uniform random trees. The expected independence ratio of a uniform random tree is the unique solution of the equation $x = e^{-x}$ (see [36]), which is approximately 0.5671..., while the greedy algorithm yields an independent set of expected density 1/2 as we will see in Section 2.3.

Finally, we note that the following parallel/distributed algorithm gives a further way to look at the maximal independent set generated by the greedy algorithm. After (randomly) ordering the vertices, we colour "red" all the *sinks*, that is, all the vertices which appear before their neighbours in the order, and then remove them and their neighbours from the graph and continue. Formulated this way, the algorithm is very easy to implement, and requires only local communication between the nodes. Also, conditioning on the initial random ordering, it is deterministic, a property which appears to be of importance (see, e.g., [6]). A main question of interest is the number of rounds it takes the algorithm to terminate. In [18] it was shown that with high probability (**whp**)[3] it terminates in $O(\ln n)$ steps on any n-vertex graph, and that this is tight. Thus, even though these algorithms may be suboptimal, they are strikingly simple and can be surprisingly efficient.

[2] The letters **iid** abbreviate "independent and identically distributed".
[3] That is, with probability tending to 1 as n tends to infinity.

1.1 Our Contribution

The goal of this work is to introduce a simple and fairly general framework for calculating the asymptotics of the greedy independence ratio for a wide variety of (random) graph sequences. The general approach is to study a suitable limiting object, typically a random rooted infinite graph, which captures the local view of a typical vertex, and to calculate the probability that its root appears in a random independent set in this graph, which is created according to some natural "local" rule, to be described later. We show that this probability approximates the expected greedy independence ratio.

Let us formulate this more precisely. For a (random) finite graph G let $\mathbf{I}(G)$ be the random greedy maximal independent set of G, let $\iota(G) := |\mathbf{I}(G)|/|V(G)|$ be its density, and let $\bar{\iota}(G)$ be its expected density (taken over the distribution of G and over the random greedy maximal independent set). Suppose (U, ρ) is a random rooted infinite graph (that is, (U, ρ) is a distribution on rooted infinite graphs). A random labelling $\sigma = (\sigma_v)_{v \in V(U)}$ of U is a process consisting of **iid** random variables σ_v, each distributed uniformly in $[0, 1]$. The past of a vertex v, denoted $\mathcal{P}_v$, is the set of vertices in U reachable from v by a monotone decreasing path (with respect to σ). We say that (U, ρ) has **nonexplosive growth** if the past of ρ is almost surely finite. For such (U, ρ) we may define

$$\iota(U, \rho) = \mathbb{P}[\rho \in \mathbf{I}(U[\mathcal{P}_\rho])],$$

where $\mathbb{P}$ denotes the probability space of the random labellings of U and $\mathbf{I}$ respects the vertex ordering induced by that random labelling.

We say that a graph sequence G_n converges locally to (U, ρ), and denote it by $G_n \xrightarrow{\text{loc}} (U, \rho)$, if for every $r \geq 0$, the ball of radius r around a uniformly chosen point from G_n converges in distribution to the ball of radius r around ρ in U. To make this notion precise, we need to endow the space of rooted locally finite connected graphs with a topology. This will be done rigorously in Section 3. The following key theorem gives motivation for the definitions above.

▶ **Theorem 1.1.** *If $G_n \xrightarrow{\text{loc}} (U, \rho)$ and (U, ρ) has nonexplosive growth then $\bar{\iota}(G_n) \to \iota(U, \rho)$.*

We remark that $\iota(U, \rho)$ is almost surely positive, implying that for locally convergent graph sequences the expected size of the random greedy maximal independent set is linear.

With some mild growth assumptions on the graph sequence, we can also obtain asymptotic concentration of the greedy independence ratio around its mean. For a graph G let $\mathcal{N}_G(r)$ be the random variable counting the number of paths of length at most r from a uniformly chosen random vertex of G. For two real numbers x, y denote by $x \wedge y$ their minimum. Let

$$\mu^*(r) = \lim_{M \to \infty} \limsup_{n \to \infty} \mathbb{E}[\mathcal{N}_{G_n}(r) \wedge M].$$

We say that G_n has subfactorial path growth (**sfpg**) if $\mu^*(r) \ll_r r!$.[4] Note that every graph sequence with uniformly bounded degrees has **sfpg**, but there are graph sequences with unbounded degrees, and even with unbounded average degree, which still have **sfpg**. For most cases, and for all of the applications presented in this paper, requiring that the somewhat simpler expression $\limsup_{n \to \infty} \mathbb{E}[\mathcal{N}_{G_n}(r)]$ is subfactorial would have sufficed; however, requiring that $\mu^*(r)$ is subfactorial is less strict, and is more natural for the following reason: if the graph sequence converges locally, then $\mu^*(r)$ is the expected number of paths of length at most r in the limit. For two functions $f_1(n), f_2(n)$ write $f_1(n) \sim f_2(n)$ if $f_1(n) = (1 + o(1)) f_2(n)$. We are now ready to state our concentration result.

[4] By $g_1(r) \ll_r g_2(r)$ we mean that $\lim_{r \to \infty} g_1(r)/g_2(r) = 0$.

▶ **Theorem 1.2.** *If G_n has **sfpg** and $G_n \xrightarrow{\text{loc}} (U,\rho)$ then $\iota(G_n) \sim \iota(U,\rho)$ with high probability.*

▶ Remark. Gamarnik and Goldberg [22] have established concentration of $\iota(G_n)$ around its mean, under the assumption that the degrees of G_n are uniformly bounded. Here we relax that assumption.

▶ Remark. A sequence of graphs which has **sfpg** does not necessarily have a local limit, but it does have a locally convergent subsequence. Any limit of such a sequence will have nonexplosive growth.

When the limiting object is supported on rooted trees, we call the (random) graph sequence **locally tree-like**. Our next result is a general differential-equations based tool for analysing the asymptotics of the greedy independence ratio of locally tree-like (random) **sfpg** graph sequences, with the restriction that their limit may be emulated by a *simple* branching process with at most countably many types. Roughly speaking, a **multitype branching process** is a rooted tree, in which each node is assigned a *type*, and the number and types of each node's "children" follow a law which depends solely on the node's type, and is independent for distinct nodes. Such a branching process is called **simple** if each such law is a product measure. Formal definitions will be given in Section 5. The following theorem reduces the problem of calculating $\iota(U,\rho)$ in these cases to the problem of solving a (possibly infinite) system of ODEs.

▶ **Theorem 1.3.** *Let (U,ρ) be a simple multitype branching process with finite or countable type set T, root distribution $\dot{\mu}$ and offspring distributions $\mu^{k\to j}$. For every $x \in [0,1]$ and $k,j \in T$ let $\mu_x^{k\to j} = \mathsf{Bin}(\mu^{k\to j}, x)$ denote the distribution of the number of children of type j of a node of type k with random label at most x. Then,*

$$\iota(U,\rho) = \sum_{k\in T} y_k(1)\dot{\mu}(k), \tag{1}$$

where $\{y_k\}_{k\in T}$ is a solution to the following system of ODEs:

$$y_k'(x) = \sum_{\ell\in\mathbb{N}^T} \prod_{j\in T} \mu_x^{k\to j}(\ell_j)\left(1 - \frac{y_j(x)}{x}\right)^{\ell_j}, \qquad y_k(0) = 0. \tag{$*$}$$

We call $(*)$ the **fundamental system of ODEs** of the branching process (U,ρ). While this system of ODEs may seem complicated, in many important cases it reduces to a fairly simple system, as we will demonstrate in Section 2. In particular, the proof of Theorem 1.3 implies that a solution to $(*)$ exists, and in the presented applications it will be unique. In the cases where (U,ρ) is either a single type branching process or a random tree with **iid** degrees, we provide an easy probability generating function tool that may be used to "skip" solving $(*)$. This is described in Appendix B. We mention that a somewhat related, but apparently less applicable statement, providing differential equations for the occupancy probability of a given vertex in bounded degree graphs, appears in [40].

▶ Remark. The proof of Theorem 1.3 actually yields a stronger statement. Replacing $y_k(1)$ with $y_k(x)$ in the RHS of (1), the obtained quantity is the probability that the root is occupied "at time x", namely, when vertices whose label is above x are ignored.

We conclude our work with a theorem, according to which on the set of all trees of a given order the expected size of the greedy MIS achieves its minimum on the path.

▶ **Theorem 1.4.** *Let $n \geq 1$, let T be a tree on n vertices and let P_n be the path on n vertices. Then $\bar{\iota}(P_n) \leq \bar{\iota}(T)$.*

This theorem gives us an exact (non-asymptotic) explicit lower bound for the expected greedy independence ratio of trees (an asymptotic upper bound is trivial). The methods used to prove it are different from the ones used in the rest of this paper, and are more combinatorial in nature. In particular, we make use of a transformation on trees, originally introduced by Csikvári in [12], which gives rise to a graded poset of all trees of a given order, in which the path is the unique minimum (say). While we are not able to show that this transformation can only increase the expected greedy independence ratio, we show it can only increase some other quantitative property of trees, which allows us to argue that paths indeed achieve the minimum expected greedy independence ratio.

1.2 Organisation of the Paper

We start by a short list of important applications in Section 2, where we prove some new results and reprove some known ones, using the machinery of Theorems 1.2 and 1.3. In a few cases, we are assisted by the claims from Appendix B. In particular, we calculate the asymptotics of the greedy independence ratio for paths and cycles (reproving results from [20, 38]), binomial random graphs (reproving a result from [35]), uniform random trees and random functional digraphs (new results) and random regular graphs or regular graphs with high girth (reproving results from [48, 33]).

We then shift our focus to the formal definitions and proofs. We begin by introducing the metric that is used to define the notion of *local convergence* in Section 3, where we also prove Theorem 1.1. In Section 4 we prove Theorem 1.2, by essentially proving a decay of correlation between vertices in terms of their distance, and showing that typical pairs of vertices are distant. In fact, the results of Section 4 imply that even without local convergence, under mild growth assumptions, the variance of the greedy independence ratio is decaying.

In Section 5 we turn our attention to locally tree-like graph sequences, define (simple, multitype) branching processes, and prove Theorem 1.3. We enhance this in Appendix B by introducing a probability generating functions based "trick", which allows, in some cases, a significant simplification. In Section 6 we focus further on tree sequences, where we prove Theorem 1.4. To this end we pinpoint several interesting properties of the expected greedy independence ratio of the path.

2 Applications

The goal of this section is to demonstrate the power of the introduced framework by finding ι for several natural (random) graph sequences, via finding their local limit and solving its fundamental system of ODEs, as described in Theorem 1.3. In some cases, we may use probability generating functions, as described in Appendix B, to ease calculations.

2.1 Infinite-Ray Stars

For $d \geq 1$, let $\mathcal{S}_d$ be the **infinite-ray star** with d branches. Formally, the vertex set of $\mathcal{S}_d$ is $\{(0,0)\} \cup \{(i,j) : i \in [d], j = 1, 2, \ldots\}$, and $(i,j) \sim (i',j')$ if $|j - j'| = 1$ and either $i = i'$ or $ii' = 0$. Note that $\mathcal{S}_1 = \mathbb{N}$ and $\mathcal{S}_2 = \mathbb{Z}$. This is a two-type branching process, with types d for the root and 1 for a branch vertex. The fundamental system of ODEs in this case is $y_d'(x) = (1 - y_1(x))^d$, and for $d = 1$ we obtain the equation $y_1' = 1 - y_1$ of which the solution is $y_1(x) = 1 - e^{-x}$. For $d > 1$ we obtain the equation $y_d' = e^{-dx}$ of which the solution is $y_d(x) = \frac{1}{d}(1 - e^{-dx})$. Since $\tau = d$ a.s., it follows that $\iota(\mathcal{S}_d) = y_d(1) = \zeta_d := \frac{1}{d}(1 - e^{-d})$. In particular, $\iota(\mathbb{N}) = 1 - e^{-1} \approx 0.6321...$ and $\iota(\mathbb{Z}) = \frac{1}{2}(1 - e^{-2}) \approx 0.43233...$.

As $\mathbb{N}$ is a single type branching process and $\mathbb{Z}$ is a random tree with **iid** degrees, we may use the alternative approach for calculating $\iota(\mathbb{N})$ and $\iota(\mathbb{Z})$, as described in Appendix B. Solving $\int_h^1 \frac{dz}{z} = 1$ gives $h = e^{-1}$, hence by Claim B.1, $\iota(\mathbb{N}) = 1 - e^{-1}$, and by Claim B.2, $\iota(\mathbb{Z}) = \frac{1}{2}\left(1 - e^{-2}\right)$.

The local limit of the sequences P_n of paths and C_n of cycles is clearly $\mathbb{Z}$. It follows from the discussion above that $\iota(P_n), \iota(C_n) \sim \frac{1}{2}(1 - e^{-2})$ **whp**. This was already calculated by Flory [20] (who only considered the expected ratio) and independently by Page [38], and can be thought of as the discrete variant of Rényi's parking constant (see [17]).

2.2 Poisson Galton–Watson Trees

A Poisson Galton–Watson tree $\mathcal{T}_\lambda$ is a single type branching process with offspring distribution $\mathsf{Pois}(\lambda)$ for some parameter $\lambda \in (0, \infty)$. The fundamental ODE in this case is $y'(x) = e^{-\lambda y(x)}$. (This can be calculated directly using (4)). The solution for this differential equation is $y(x) = \ln(1+\lambda x)/\lambda$, hence $\iota(\mathcal{T}_\lambda) = y(1) = \ln(1+\lambda)/\lambda$. The same result can be obtained using the probability generating function of the Poisson distribution, as described in Appendix B.

Consider the **binomial random graph** $G(n, \lambda/n)$, which is the graph on n vertices in which every pair of nodes is connected by an edge independently with probability λ/n. It is easy to check that it converges locally to $\mathcal{T}_\lambda$, hence $\iota(G(n, \lambda/n)) \sim \ln(1 + \lambda)/\lambda$ **whp**, recovering a known result (see [35]).

2.3 Size-Biased Poisson Galton–Watson Trees

For $0 < \lambda \leq 1$, a size-biased Poisson Galton–Watson tree $\hat{\mathcal{T}}_\lambda$ can be defined (see [34]) as a two-type simple branching process, with types s (*spine* vertices) and t (*tree* vertices), where a spine vertex has 1 spine child plus $\mathsf{Pois}(\lambda)$ tree children, a tree vertex has $\mathsf{Pois}(\lambda)$ tree children, and the root is a spine vertex. The fundamental system of ODEs in this case is

$$\begin{aligned} y_{\mathsf{s}}'(x) &= x \sum_{d=0}^{\infty} \frac{(\lambda x)^d}{e^{\lambda x} d!} \left(1 - \frac{y_{\mathsf{s}}(x)}{x}\right)\left(1 - \frac{y_{\mathsf{t}}(x)}{x}\right)^d + (1 - x) \sum_{d=0}^{\infty} \frac{(\lambda x)^d}{e^{\lambda x} d!} \left(1 - \frac{y_{\mathsf{t}}(x)}{x}\right)^d \\ &= (1 - y_{\mathsf{s}}(x)) \sum_{d=0}^{\infty} \frac{(\lambda x)^d}{e^{\lambda x} d!} \left(1 - \frac{y_{\mathsf{t}}(x)}{x}\right)^d = (1 - y_{\mathsf{s}}(x)) e^{-\lambda y_{\mathsf{t}}(x)}, \end{aligned}$$

and from Section 2.2 we obtain $y_{\mathsf{t}}(x) = \ln(1 + \lambda x)/\lambda$. Hence $y_{\mathsf{s}}'(x) = (1 - y_{\mathsf{s}}(x))/(1 + \lambda x)$, and the solution for that equation is $y_{\mathsf{s}}(x) = 1 - \exp(-\ln(1 + \lambda x)/\lambda)$. Thus $\iota(\hat{\mathcal{T}}_\lambda) = y_{\mathsf{s}}(1) = 1 - (1 + \lambda)^{-1/\lambda} = 1 - e^{-\iota(\mathcal{T}_\lambda)}$. In particular, $\iota(\hat{\mathcal{T}}_1) = 1/2$.

It is a classical (and beautiful) fact (see, e.g., [32, 24]) that if T_n is a uniformly chosen random tree drawn from the set of n^{n-2} trees on (labelled) n vertices, then T_n converges locally to $\hat{\mathcal{T}}_1$, hence $\iota(T_n) \sim 1/2$ **whp**. To the best of our knowledge, this intriguing fact was not previously known. In fact, it was shown recently in [27] that if G_n is a sequence of connected regular graphs that converges to a nondegenerate graphon, and T_n is the uniform spanning tree of G_n, then T_n also converges locally to $\hat{\mathcal{T}}_1$, hence it follows that $\iota(T_n) \sim 1/2$ **whp** in this case as well.

It can be easily verified that the local limit of a random functional digraph $\vec{G}_1(n)$ (the digraph on n vertices whose edges are $(i, \pi(i))$ for a uniform random permutation π), with orientations ignored, is also $\hat{\mathcal{T}}_1$, hence $\iota(\vec{G}_1) \to 1/2$ **whp**.

2.4 d-ary Trees

For $d > 1$, let T_d be the d-ary tree. It may be viewed as a (single type) branching process. It thus immediately follows from (4) that $y'(x) = (1 - y(x))^d$. The solution for this differential equation is $y(x) = 1 - ((d-1)x + 1)^{-1/(d-1)}$. It follows that $\iota(\mathsf{T}_d) = y(1) = 1 - d^{-1/(d-1)}$. This fact also follows easily using the generating functions approach described in Appendix B. A remarkable example is $\iota(\mathsf{T}_2) = 1/2$.

2.5 Regular Trees

For $d \geq 3$, let $\mathbb{T}_d$ be the d-regular tree. It may viewed as a two-type branching process with types d for the root and 1 for the rest of the vertices. The fundamental system of ODEs in this case is $y_d'(x) = (1 - y_1(x))^d$, and from Section 2.4 we obtain $y_1(x) = 1 - ((d-2)x+1)^{-1/(d-2)}$. It follows that $y_d'(x) = ((d-2)x+1)^{-d/(d-2)}$, of which the solution is $y_d(x) = (1 - ((d-2)x + 1)^{-2/(d-2)})/2$. Therefore,

$$\iota(\mathbb{T}_d) = y_d(1) = \frac{1}{2}\Big(1 - (d-1)^{-2/(d-2)}\Big).$$

As with d-ary trees, here again the generating functions approach works easily: the solution to $\int_{h(x)}^{1} z^{d-1} dz = x$ is $h(x) = (1 - (2-d)x)^{1/(2-d)}$, and the result follows from Claim B.2. Remarkable examples include $\iota(\mathbb{T}_3) = 3/8$ and $\iota(\mathbb{T}_4) = 1/3$.

Since the **random regular graph** $G(n, d)$ (a uniformly sampled graph from the set of all d-regular graphs on n vertices, assuming dn is even) converges locally to $\mathbb{T}_d$ (see, e.g., [50]), the above result for this case is exactly [48, Theorem 4]. In fact, since any sequence of d-regular graphs with girth tending to infinity converges locally to $\mathbb{T}_d$, we also recover [33, Theorem 2].

3 Local Limits

In order to study asymptotics, it is often useful to construct a suitable limiting object first. Local limits were introduced by Benjamini and Schramm [3] and studied further by Aldous and Steele [2] (A very similar approach has already been introduced by Aldous in [1]). Local limits, when they exist, encapsulate the asymptotic data of local behaviour of the convergent graph sequence, and in particular, that of the performance of the greedy algorithm.

We start with basic definitions. Consider the space $\mathcal{G}_\bullet$ of rooted locally finite connected graphs viewed up to root preserving graph isomorphisms. We provide $\mathcal{G}_\bullet$ with the metric $d_{\text{loc}}((G_1, \rho_1), (G_2, \rho_2)) = 2^{-R}$, where R is the largest integer for which $B_{G_1}(\rho_1, R) \simeq B_{G_2}(\rho_2, R)$. Here we understand $B_G(\rho, R)$ as the *rooted* subgraph of (G, ρ) spanned by the vertices of distance at most R from ρ, and $\simeq$ as *rooted-isomorphic*. It is an easy fact that $(\mathcal{G}_\bullet, d_{\text{loc}})$ is a separable complete metric space, hence it is a Polish space. $(\mathcal{G}_\bullet, d_{\text{loc}})$, while being bounded, is not compact (the sequence of rooted stars S_n does not have a convergent subsequence).

Recall that a sequence of random elements $\{X_n\}_{n=1}^{\infty}$ **converges in distribution** to a random element X, if for every bounded continuous function f we have that $\mathbb{E}[f(X_n)] \to \mathbb{E}[f(X)]$. Let G_n be a sequence of (random) finite graphs. We say that G_n **converges locally** to a (random) element (U, ρ) of $\mathcal{G}_\bullet$ if for every $r \geq 0$, the sequence $B_{G_n}(\rho_n, r)$ converges in distribution to $B_U(\rho, r)$, where ρ_n is a uniformly chosen vertex of G_n. Since the inherited topology on all rooted balls in $\mathcal{G}_\bullet$ with radius r is discrete, this implies convergence in total variation distance.

We are now ready to prove Theorem 1.1.

Proof of Theorem 1.1. Fix $\varepsilon > 0$. For a given labelling σ of U, let ℓ_σ be the length of the longest decreasing sequence (w.r.t. σ) starting from ρ. Since (U, ρ) has nonexplosive growth, there exists r_ε for which for every $r \geq r_\varepsilon$, $\mathbb{P}[\ell_\sigma \geq r] < \varepsilon$. For $r \geq 0$, let $G_n^r = B_{G_n}(\rho_n, r)$ and $U^r = B_U(\rho, r)$. We couple G_n^r and a random permutation π on its vertices with U^r and a random labelling σ as follows. First, since G_n^r converges in distribution (and hence in total variation distance) to U^r, there exists n_r such that for all $n \geq n_r$ we have that $\mathbb{P}[G_n^r \not\cong U^r] \leq \varepsilon$. If this event occurs, we say that the coupling has failed. Otherwise, for some isomorphism $\varphi : G_n^r \to U^r$, we let π be the permutation on the vertices of G_n^r which agrees with the ordering of the labels on the vertices of the isomorphic image (that is, $\pi_u < \pi_v \iff \sigma_{\varphi(u)} < \sigma_{\varphi(v)}$). Note that under this coupling, if it succeeds, $\rho_n \in \mathbf{I}(G_n^r) \iff \rho \in \mathbf{I}(U^r)$. However, on the event "$\ell_\sigma \leq r$", $\rho_n \in \mathbf{I}(G_n^r) \iff \rho_n \in \mathbf{I}(G_n)$ and $\rho \in \mathbf{I}(U^r) \iff \rho \in \mathbf{I}(U[\mathcal{P}_\rho])$. Observing that $\bar{\iota}(G_n) = \mathbb{P}[\rho_n \in \mathbf{I}(G_n)]$ we obtain that for $r \geq r_\varepsilon$ and $n \geq n_r$, $|\bar{\iota}(G_n) - \iota(U, \rho)| < 2\varepsilon$. ◀

4 Concentration

With some mild growth assumptions on the graph sequence, without assuming local convergence, we obtain asymptotic concentration of the greedy independence ratio around its mean. Under these assumptions we show that the dependence between the inclusion of distinct nodes in the maximal independent set decays as a functions of their distance, a phenomenon which is sometimes called *correlation decay* or *long-range independence*. To prove that the model exhibits this phenomenon, we show that with high probability there are no "long" monotone paths emerging from a typical vertex, which is the contents of the next claim. We then observe that two independent random vertices are typically distant, and use a general lemma about exploration algorithms to prove decay of correlation. We remark that similar locality arguments appear in [37]. Some of the proofs are given in Appendix A.

▷ Claim 4.1. Suppose that G_n has **sfpg**. Let π be a uniform random permutation of the vertices of G_n, and let u be a uniformly chosen vertex from G_n. Then, for every $\varepsilon > 0$, there exists $r > 0$ such that for every large enough n, the probability that there exists a monotone decreasing path of length r (w.r.t. π), emerging from u, is at most ε.

▷ Claim 4.2. Suppose that G_n has **sfpg**. Let u, v be two independently and uniformly chosen vertices from G_n. Then, for every $\varepsilon, r \geq 0$ we have that for every large enough n, $\mathbb{P}[\mathrm{dist}_{G_n}(u, v) \leq r] \leq \varepsilon$.

Let $G = (V, E)$ be a graph. An **exploration-decision rule** for G is a (deterministic) function $\mathcal{Q}$, whose input is a pair (S, g), where S is a non-empty sequence of distinct vertices of V, and $g : S \to [0, 1]$, and whose output is either a vertex $v \in V \setminus S$ or a "decision" T or F. An **exploration-decision algorithm** for G, with rule $\mathcal{Q}$, is a (deterministic) algorithm A, whose input is an initial vertex $v \in V$ and a function $f : V \to [0, 1]$, which outputs T or F, and operates as follows. Set $u_1 = v$. Suppose A has already set $u_1, \ldots, u_i$. Let $x = \mathcal{Q}((u_1, \ldots, u_i), f\restriction_{\{u_1, \ldots, u_i\}})$. If $x \in V$, set $u_{i+1} = x$ and continue. Otherwise stop and return x. We call the set $u_1, \ldots, u_i$ at this stage the **range** of the algorithm's run. We denote the output of the algorithm by $\mathsf{A}(v, f)$ and its range by $\mathrm{rng}_{\mathsf{A}}(v, f)$. The radius of the algorithm's run, denoted $\mathrm{rad}_{\mathsf{A}}(v, f)$, is the maximum distance between v and an element of its range.

▶ **Lemma 4.3.** *Let $\varepsilon > 0$. Let $G = (V, E)$ be a graph, let σ be a random labelling of its vertices, let A be an exploration-decision algorithm for G and let $r \geq 1$. Let u, v be sampled independently from some distribution over V. Suppose that w.p. at least $1 - \varepsilon$ both $\mathrm{dist}_G(u, v) \geq 3r$, and $\mathrm{rad}_{\mathsf{A}}(u, \sigma), \mathrm{rad}_{\mathsf{A}}(v, \sigma) \leq r$. Then $|\mathrm{cov}[\mathsf{A}(u, \sigma), \mathsf{A}(v, \sigma)]| = o_\varepsilon(1)$.*

We now apply the lemma in our setting.

▷ Claim 4.4. Suppose that G_n has **sfpg**. Let u, v be two independently and uniformly chosen vertices from G_n. Denote by R_u, R_v the events that $u \in \mathbf{I}(G_n)$, $v \in \mathbf{I}(G_n)$, respectively. Then $|\operatorname{cov}[R_u, R_v]| = o(1)$.

Proof. Let $\varepsilon > 0$. We describe an exploration-decision algorithm A by defining its rule. Given a vertex sequence $S = (u_1, \ldots, u_i)$ and labels $g : S \to [0,1]$, the rule checks for monotone decreasing sequences emerging from u_1, in S, with respect to g. Denote by $\mathcal{E}$ the set of ends of these sequences. If there are vertices in $V \setminus S$ with neighbours in $\mathcal{E}$, return an arbitrary vertex among these. Otherwise, perform the Greedy MIS algorithm on the past of u_1 inside S, and return T if u_1 ends up in the MIS, or F otherwise. We observe that if σ is a random labelling of G_n then for $w \in \{u, v\}$ the event $\mathsf{A}(w, \sigma) = \mathsf{T}$ is in fact the event R_w. We also note that if the longest monotone decreasing sequence, w.r.t. σ, emerging from w is of length $r - 1$, then $\operatorname{rad}_{\mathsf{A}}(w, \sigma) \leq r$.

By Claim 4.1 there exists $r > 0$ such that for every large enough n the probability that there exists a monotone decreasing path of length $r - 1$ from either u or v is at most ε. By Claim 4.2, for large enough n, the probability that the distance between u and v is at most $3r$ is at most ε. Therefore, by Lemma 4.3, $|\operatorname{cov}[\mathsf{A}(u, \sigma), \mathsf{A}(v, \sigma)]| = o_\varepsilon(1)$. ◁

▷ Claim 4.5. Suppose that G_n has **sfpg**. Then $\operatorname{Var}[\iota(G_n)] = o(1)$.

Proof. For a vertex w, denote by R_w the event that $w \in \mathbf{I}(G_n)$. Let u, v be two independently and uniformly chosen vertices from G_n. Since the random variables $\mathbb{E}[R_u \mid u]$ and $\mathbb{E}[R_v \mid v]$ are independent, by Claim 4.4,

$$\begin{aligned}\operatorname{Var}[\iota(G_n)] &= \mathbb{E}[\operatorname{cov}[R_u, R_v \mid u, v]] \\ &= \operatorname{cov}[R_u, R_v] - \operatorname{cov}[\mathbb{E}[R_u \mid u]\mathbb{E}[R_v \mid v]] = \operatorname{cov}[R_u, R_v] = o(1).\end{aligned}$$ ◁

Proof of Theorem 1.2. Let $\varepsilon > 0$. Note that since G_n has **sfpg**, (U, ρ) has nonexplosive growth, hence by Theorem 1.1 there exists n_0 such that for every $n \geq n_0$, $|\bar{\iota}(G_n) - \iota(U, \rho)| \leq \varepsilon$. Thus, by Chebyshev's inequality and Claim 4.5,

$$\mathbb{P}[|\iota(G_n) - \iota(U, \rho)| > 2\varepsilon] \leq \mathbb{P}[|\iota(G_n) - \bar{\iota}(G_n)| > \varepsilon] \leq \varepsilon^{-2} \operatorname{Var}[\iota(G_n)] = o(1).$$ ◀

5 Branching Processes and Differential Equations

As promised, we begin with a formal definition of multitype branching processes. Let T be a finite or countable set, which we call the **type set**. Let $\dot{\mu}$ be a distribution on T, which we call the **root distribution**, and for each $k \in T$ let $(\mu^{k \to j})_{j \in T}$ be an **offspring distribution**, which is a distribution on vectors with nonnegative integer coordinates. Let $\tau \sim \dot{\mu}$ and for every finite sequence of natural numbers $\mathbf{v}$ let $(\xi_{\mathbf{v}}^{k \to j})_{j \in T} \sim (\mu^{k \to j})_{j \in T}$ be a random vector, where these random vectors are independent for different indices $\mathbf{v}$ and are independent of τ. A **multitype branching process** $(\mathbf{Z}_t)_{t \in \mathbb{N}}$ with type set T, root distribution $\dot{\mu}$ and offspring distributions $(\mu^{k \to j})_{j \in T}$ is a Markov process on labelled trees, in which each vertex is assigned a type in T, which may be described as follows. At time $t = 0$ the tree $\mathbf{Z}_0$ consists of a single vertex of type τ, labelled by the empty sequence. At time $t + 1$ the tree $\mathbf{Z}_{t+1}$ is obtained from $\mathbf{Z}_t$ as follows. For each $k \in T$ and $\mathbf{v}$ of length t and type k in $\mathbf{Z}_t$, we add the vertices $\mathbf{v} \frown i$ for all $0 \leq i < \sum_{j \in T} \xi_{\mathbf{v}}^{k \to j}$, having exactly $\xi_{\mathbf{v}}^{k \to j}$ of them being assigned type j, uniformly at random, and connecting them with edges to $\mathbf{v}$.[5] If in addition $(\mu^{k\to j})_{j\in T}$ is a product measure, namely, if $\xi_{\mathbf{v}}^{k\to j} \sim \mu^{k\to j}$ are sampled independently for distinct $j \in T$, the process is called **simple**. We often think of a multitype branching process as the possibly infinite (random) rooted graph $\mathbf{Z}_\infty = \bigcup_{t\geq 0} \mathbf{Z}_t$, rooted at the single vertex of $\mathbf{Z}_0$.

Proof of Theorem 1.3. Let σ be a random labelling of U. To ease notation, set $\iota = \iota(U, \rho)$ and $\mathbf{I} = \mathbf{I}(U[\mathcal{P}_\rho])$, and recall that $\iota = \mathbb{P}[\rho \in \mathbf{I}]$. Let $\tau \sim \dot{\mu}$ be the type of the root. For $k \in T$ and $x \in [0,1]$, define $\iota^{(k)} = \mathbb{P}[\rho \in \mathbf{I} \mid \tau = k]$ and $\iota_x^{(k)} = \mathbb{P}[\rho \in \mathbf{I} \mid \sigma_\rho = x,\ \tau = k]$. Note that this is well defined, even if the event that $\sigma_\rho = x$ has probability 0. Let further

$$\iota_{<x}^{(k)} = \int_0^x \iota_z^{(k)} dz,$$

so $\iota^{(k)} = \iota_{<1}^{(k)}$, hence

$$\iota = \sum_{k\in T} \iota_{<1}^{(k)} \cdot \mathbb{P}[\tau = k].$$

It therefore suffices to show that the family $y_k(x) := \iota_{<x}^{(k)}$ satisfies $(*)$ (it clearly satisfies the boundary conditions). The key observation is that distinct children in the past of the root are roots to independent subtrees. Formally, conditioning on the event that $v_1, \ldots, v_a$ are the children of ρ in its past, the events "$v_i \in \mathbf{I}$" for $i = 1, \ldots, a$ are mutually independent. Since $\rho \in \mathbf{I}$ if and only if $v_i \notin \mathbf{I}$ for every $i = 1, \ldots, a$,

$$\begin{aligned} y_k'(x) = (\iota_{<x}^{(k)})' = \iota_x^{(k)} &= \sum_{\ell\in\mathbb{N}^T} \prod_{j\in T} \mu_x^{k\to j}(\ell_j)(1 - \mathbb{P}[\rho \in \mathbf{I} \mid \sigma_\rho < x,\ \tau = j])^{\ell_j} \\ &= \sum_{\ell\in\mathbb{N}^T} \prod_{j\in T} \mu_x^{k\to j}(\ell_j)\left(1 - \frac{y_j(x)}{x}\right)^{\ell_j}. \end{aligned}$$

◀

6 Lower Bound on Tree Sequences

Let us focus on tree sequences. How large can the expected greedy independent ratio be? How small can it be? The sequence of stars is a clear witness that the only possible asymptotic upper bound is the trivial one, namely 1. Apparently, the lower bound is not trivial. An immediate corollary of Theorems 1.1 and 1.4 is that a tight asymptotic lower bound is $\iota(\mathbb{Z}) = (1 - e^{-2})/2$ (compare with [44]). The statement of Theorem 1.4 is, however, much stronger: paths achieve the *exact* (non-asymptotic) lower bound for the expected greedy independence ratio among the set of all trees of a given order.

To prove Theorem 1.4 we will need to first understand the behaviour of the greedy algorithm on the path.

For a graph G denote by $\mathfrak{i}(G)$ the cardinality of its greedy independent set, and let $\bar{\mathfrak{i}}(G) = \mathbb{E}[\mathfrak{i}(G)]$. Let $\alpha_n = \bar{\mathfrak{i}}(P_n)$. Suppose the vertices of P_n are $1, \ldots, n$, and let S be the vertex which is first in the permutation of the vertices. Setting $\alpha_{-1} = \alpha_0 = 0$, we obtain the recursion

$$\alpha_n = \mathbb{E}[\mathbb{E}[\mathfrak{i}(P_n) \mid S]] = \frac{1}{n}\sum_{i=1}^{n}(1 + \alpha_{i-2} + \alpha_{n-i-1}) = 1 + \frac{2}{n}\sum_{i=1}^{n}\alpha_{i-2}, \tag{2}$$

[5] By $\mathbf{v}^\frown i$ we mean the sequence obtained from $\mathbf{v}$ by appending the element i.

from which an explicit formula for α_n can be derived (see [21]). We will need the following two properties of α_n, whose proofs (which are rather long and technical) we omit in this extended abstract.

▷ Claim 6.1. α_n is monotone increasing and subadditive.

Let $\xi_{n,\ell} = \sum_{j=1}^{\ell} \alpha_{n+j}$.

▷ Claim 6.2. For every $\ell, a, b \geq 1$ it holds that $\xi_{a,\ell} + \xi_{b,\ell} \leq \xi_{a+b,\ell} + \xi_{0,\ell}$.

6.1 KC-Transformations

In this section we introduce the main tool that will be used to prove Theorem 1.4. Let T be a tree and let x, y be two vertices of T. We say that the path between x and y is **bare** if for every vertex $v \neq x, y$ on that path, $d_T(v) = 2$. Suppose x, y are such that the unique path P in T between them is bare, and let z be the neighbour of y in that path. For a vertex v, denote by $N(v)$ the neighbours of v in T. The **KC-transformation** $\mathrm{KC}(T, x, y)$ of T with respect to x, y is the tree obtained from T by deleting every edge between y and $N(y) \setminus z$ and adding the edges between x and $N(y) \setminus z$ instead. Note that $\mathrm{KC}(T, x, y) \simeq \mathrm{KC}(T, y, x)$, so if we care about unlabelled trees, we may simply write $\mathrm{KC}(T, P)$, for a bare path P in T. The term "KC-transformation" was coined by Bollobás and Tyomkyn [10] after Kelmans, who defined a similar operation on graphs [31], and Csikvári, who defined it in this form [12] under the name "generalized tree shift" (GTS).

A nice property of KC-transformations, first observed by Csikvári [12], is that they induce a graded poset on the set of unlabelled trees of a given order, which is graded by the number of leaves. In particular, this means that in that poset, the path is the unique minimum (say) and the star is the unique maximum. Note that if P contains a leaf then $\mathrm{KC}(T, P) \simeq T$, and otherwise $\mathrm{KC}(T, P)$ has one more leaf than T. In the latter case, we say that the transformation is **proper**.

Here is the plan for how to prove Theorem 1.4. For a tree T and a vertex v, denote by $T \star v$ the forest obtained from T by **shattering** T at v, that is, by removing from T the set $\{v\} \cup N(v)$. Denote by $\kappa_v(T)$ the multiset of orders of trees in the forest $T \star v$, and by $\kappa(T)$ the sum of $\kappa_v(T)$ for all vertices v in T. Note that for trees with up to 3 vertices, Theorem 1.4 is trivial; we proceed by induction. By the induction hypothesis,

$$\bar{\mathrm{i}}(T) = \frac{1}{n} \sum_{v \in V(T)} \sum_{S \in T \star v} (1 + \bar{\mathrm{i}}(S)) \geq 1 + \frac{1}{n} \sum_{v \in V(T)} \sum_{k \in \kappa_v(T)} \alpha_k = 1 + \frac{1}{n} \sum_{k \in \kappa(T)} \alpha_k. \tag{3}$$

Therefore, it makes sense to study the quantities $\nu_v(T) = \sum_{k \in \kappa_v(T)} \alpha_k$ and $\nu(T) = \sum_{k \in \kappa(T)} \alpha_k$. In fact, it would suffice to show that for any tree T on n vertices $\nu(T) \geq \nu(P_n)$, since by (2) and (3) we would obtain

$$\bar{\mathrm{i}}(T) \geq 1 + \frac{1}{n} \nu(T) \geq 1 + \frac{1}{n} \nu(P_n) = \bar{\mathrm{i}}(P_n).$$

We therefore reduced our problem to proving the following theorem about KC-transformations.

▶ **Theorem 6.3.** *If T is a tree and P is a bare path in T then $\nu(\mathrm{KC}(T, P)) \geq \nu(T)$.*

It would have been nice if for every $v \in V(T)$ we would have had $\nu_v(\mathrm{KC}(T, P)) \geq \nu_v(T)$; unfortunately, this is not true in general. However, the following statement, whose proof can be found in Appendix C, would suffice.

▶ **Theorem 6.4.** *Let T be a tree and let $x \neq y$ be two vertices with the path between them being bare. Denote $T' = \mathrm{KC}(T, x, y)$. Let A be the set of vertices $v \neq x$ in T for which every path between v and y passes via x, and similarly, let B be the set of vertices $v \neq y$ in T for which every path between v and x passes via y. Let P be the set of vertices on the bare path between x and y, so $A \cup B \cup P$ is a partition of $V(T)$. Then*

1. *For $v \in A \cup B$ we have that $\nu_v(T') \geq \nu_v(T)$.*
2. $\sum_{v \in P} \nu_v(T') \geq \sum_{v \in P} \nu_v(T)$.

7 Concluding Remarks and Open Questions

Non Locally Tree-Like Graph Sequences

Our local limit approach does not assume that the converging sequence is locally tree-like. However, the differential equation tool fails completely if short cycles appear in a typical local view. As it seems, to date, there is no general tool to handle these cases, and indeed, even the asymptotic behaviour of the random greedy MIS algorithm on d-dimensional tori (for $d \geq 2$) remains unknown.

Better Local Rules

The random greedy algorithm presented here follows a very simple local rule. More complicated local rules may yield, in some cases, larger maximal independent sets; for example, the initial random ordering may "favour" low degree vertices. It would be nice to adapt our framework, or at least some of its components, to other settings. For *adaptive* "better" local algorithms we refer the reader to [48, 51].

The Second Colour

In this work we have analysed the output of the random greedy algorithm for producing a maximal independent set. As already remarked, this is in fact the set of vertices in the first colour class in the random greedy colouring algorithm. It is rather easy to see, that, after slight modifications (in particular, in Theorem 1.3) this approach allow us to calculate the asymptotic proportion of the size of the set of vertices in the second colour class (or in the k'th colour class in general, for any fixed k) as well. Non-asymptotic questions about the expected cardinality of the set of vertices in the second colour class might be also of interest. For example, is it true that the path has the smallest expected number of vertices in the first two colour classes among all trees of the same order? It is not hard to see that this statement is not true for the first three colour classes (as three colours suffice to greedily colour the path).

Monotonicity With Respect to KC-Transformations

It is likely that the expected greedy independence ratio in trees is monotone with respect to KC-transformations, and strictly monotone with respect to *proper* KC-transformations. If true, this would imply that the greedy independence ratio in trees achieves its unique minimum on the path and its unique maximum on the star.

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A Proofs for Section 4

Proof of Claim 4.1. Let $\varepsilon \geq 0$. Since $\mu^*(r) \ll_r r!$ for every large enough r we have $\mu^*(r) \leq \varepsilon r!$. We couple $\mathcal{N}_{G_n}(r)$ and u such that the former counts the number of paths of length at most r emerging from the latter. Denote by A_n^r the event that there exists a monotone decreasing path in G_n (w.r.t. π) emerging from u of length r. Note that the probability that a given path of length r is monotone decreasing w.r.t. π is $1/r!$. Since $\mu^*(r)$ is finite, there exists $M \geq 0$ such that $\mathbb{P}[\mathcal{N}_{G_n}(r) > M] < \varepsilon$ for every large enough n. In addition, for large enough n we have $\mathbb{E}[\mathcal{N}_{G_n}(r) \wedge M] \leq 2\mu^*(r)$. Hence, for large enough n,

$$\begin{aligned}\mathbb{P}[A_n^r] &\leq \sum_{m=0}^{M} \mathbb{P}[A_n^r \mid \mathcal{N}_{G_n}(r) = m] \cdot \mathbb{P}[\mathcal{N}_{G_n}(r) = m] + \mathbb{P}[\mathcal{N}_{G_n}(r) > M] \\ &\leq \frac{1}{r!} \cdot \mathbb{E}[\mathcal{N}_{G_n}(r) \wedge M] + \varepsilon \leq 3\varepsilon. \end{aligned}$$ ◁

Proof of Claim 4.2. Let $\varepsilon, r \geq 0$. We couple $\mathcal{N}_{G_n}(r)$ and u such that the former counts the number of paths of length at most r emerging from the latter. Note that under this coupling, $|B_{G_n}(u,r)| \leq \mathcal{N}_{G_n}(r)$. Since $\mu^*(r)$ is finite, there exists $M \geq 0$ such that $\mathbb{P}[\mathcal{N}_{G_n}(r) > M] < \varepsilon$ for every large enough n. Hence, for large enough n,

$$
\begin{aligned}
&\mathbb{P}[\mathrm{dist}_{G_n}(u,v) \le r] = \mathbb{P}[v \in B_{G_n}(u,r)] \\
&\le \sum_{m=0}^{M} \mathbb{P}[v \in B_{G_n}(u,r) \mid \mathcal{N}_{G_n}(r) = m] \cdot \mathbb{P}[\mathcal{N}_{G_n}(r) = m] + \mathbb{P}[\mathcal{N}_{G_n}(r) > M] \\
&\le \frac{1}{n} \cdot \mathbb{E}[\mathcal{N}_{G_n}(r) \wedge M] + \varepsilon \le \frac{M}{n} + \varepsilon \le 2\varepsilon. \qquad \triangleleft
\end{aligned}
$$

▶ Remark. We only used the fact that $\mathcal{N}_{G_n}(r)$ are uniformly integrable for every $r \ge 0$.

Proof of Lemma 4.3. Let $\mathcal{Q}$ be the rule of the algorithm A. The r**-truncated** version of $\mathcal{Q}$, denoted $\mathcal{Q}^r$, is defined as follows. To determine $\mathcal{Q}^r((u_1,\dots,u_i),g)$, $\mathcal{Q}^r$ checks the value $x = \mathcal{Q}((u_1,\dots,u_i),g)$. If $x \in \{\mathsf{T},\mathsf{F}\}$ or $\mathrm{dist}_G(u_1,x) \le r$, $\mathcal{Q}$ returns x. Otherwise it returns F. The r**-truncated** version of the algorithm A, denoted A^r, is the exploration-decision algorithm with rule $\mathcal{Q}^r$. Note that for every v and f, $\mathrm{rad}_{\mathsf{A}^r}(v,f) \le r$.

For a vertex $w \in \{u,v\}$, let X_w be the event "$\mathsf{A}(w,\sigma) = \mathsf{T}$", let Y_w be the event "$\mathsf{A}^r(w,\sigma) = \mathsf{T}$", and let $r_w = \mathrm{rad}_{\mathsf{A}}(w,\sigma)$. Note that $\mathbb{P}[X_w \wedge r_w \le r] = \mathbb{P}[Y_w \wedge r_w \le r] = \mathbb{P}[Y_w]$, thus $\mathbb{P}[X_w] = \mathbb{P}[Y_w] + o_\varepsilon(1)$. Since for x,y satisfying $\mathrm{dist}_G(x,y) \ge 3r$ we have that Y_x, Y_y are independent, it follows that $\mathbb{P}[Y_u \wedge Y_v] = \mathbb{P}[Y_u]\mathbb{P}[Y_v] + o_\varepsilon(1)$.

$$
\begin{aligned}
\mathbb{P}[X_u \wedge X_v] &= \mathbb{P}[X_u \wedge X_v \wedge (\max\{r_u,r_v\} \le r)] + \mathbb{P}[X_u \wedge X_v \wedge (\max\{r_u,r_v\} > r)] \\
&= \mathbb{P}[Y_u \wedge Y_v \wedge (\max\{r_u,r_v\} \le r)] + o_\varepsilon(1) \\
&= \mathbb{P}[Y_u \wedge Y_v] + o_\varepsilon(1) = \mathbb{P}[Y_u]\mathbb{P}[Y_v] + o_\varepsilon(1) = \mathbb{P}[X_u]\mathbb{P}[X_v] + o_\varepsilon(1). \qquad \blacktriangleleft
\end{aligned}
$$

B Probability Generating Functions

The goal of this section is to demonstrate how generating functions may aid solving the fundamental system of ODEs $(*)$ (and thus finding ι) for certain simple branching processes. In the following sections, we will use the notation $y_k(x)$ as in $(*)$, and omit the subscript k when the branching process has a single type.

Single Type Branching Processes

For a probability distribution $\mathbf{p} = (p_d)_{d=0}^{\infty}$, let $\mathsf{T}_{\mathbf{p}}$ be the $\mathbf{p}$-ary tree, namely, it is a (single type) branching process, for which the offspring distribution is $\mathbf{p}$. The fundamental ODE in this case is

$$
y'(x) = \sum_{d=0}^{\infty} p_d \sum_{\ell=0}^{d} \binom{d}{\ell} (1-x)^{d-\ell} x^{\ell} \left(1 - \frac{y(x)}{x}\right)^{\ell} = \sum_{d=0}^{\infty} p_d (1 - y(x))^d. \tag{4}
$$

This differential equation may not be solvable, but in many important cases it is, and we will use it. Denote by $g_{\mathbf{p}}(z)$ the probability generating function (**pgf**) of $\mathbf{p}$, that is,

$$
g_{\mathbf{p}}(z) = \sum_{d=0}^{\infty} p_d z^d. \tag{5}
$$

Let $\mathsf{h}_{\mathbf{p}}(x)$ be the solution to the equation

$$
\int_{\mathsf{h}_{\mathbf{p}}(x)}^{1} \frac{dz}{g_{\mathbf{p}}(z)} = x. \tag{6}
$$

▷ Claim B.1. $y(x) = 1 - \mathsf{h}_{\mathbf{p}}(x)$.

Proof. Fix $x \in [0,1]$, let $\mathsf{h} = \mathsf{h}_{\mathbf{p}}(x)$ and $g(z) = g_{\mathbf{p}}(z)$. Define $\varphi : [0,\beta] \to [\mathsf{h},1]$, where $\beta = y^{-1}(1-\mathsf{h})$, as follows: $\varphi(u) = 1 - y(u)$. Note that by (4),

$$\varphi'(u) = -y'(u) = -g(\varphi(u)).$$

Thus

$$x = \int_{\mathsf{h}}^{1} \frac{dz}{g(z)} = -\int_{\varphi(0)}^{\varphi(\beta)} \frac{dz}{g(z)} = -\int_{0}^{\beta} \frac{\varphi'(z)dz}{g(\varphi(z))} = \beta,$$

hence $y(x) = 1 - \mathsf{h}$. ◁

In particular, it follows from Claim B.1 that $\iota(\mathsf{T}_{\mathbf{p}}) = 1 - \mathsf{h}_{\mathbf{p}}(1)$.

Random Trees With IID Degrees

For a probability distribution $\mathbf{p} = (p_d)_{d=1}^{\infty}$, let $\mathbb{T}_{\mathbf{p}}$ be the **p**-tree, namely, it is a random tree in which the degrees of the vertices are independent random variables with distribution p. We may view it as a two-type branching process, with type 0 for the root and 1 for the rest of the vertices. Let $g_{\mathbf{p}}(z)$ be the **pgf** of **p** (see (5), and note that $p_0 = 0$). The fundamental system of ODEs in this case is

$$y_0'(x) = \sum_{d=1}^{\infty} p_d \sum_{\ell=0}^{d} \binom{d}{\ell} (1-x)^{d-\ell} x^{\ell} \left(1 - \frac{y_1(x)}{x}\right)^{\ell} = \sum_{d=1}^{\infty} p_d (1 - y_1(x))^d = g_{\mathbf{p}}(1-y_1(x)), \tag{7}$$

and by (4),

$$y_1'(x) = \sum_{d=0}^{\infty} p_{d+1}(1-y_1(x))^d = \frac{1}{1-y_1(x)} \sum_{d=1}^{\infty} p_d (1-y_1(x))^d = \frac{g_{\mathbf{p}}(1-y_1(x))}{1-y_1(x)}. \tag{8}$$

Let $\mathfrak{h}_{\mathbf{p}}(x)$ be the solution to the equation

$$\int_{\mathfrak{h}_{\mathbf{p}}(x)}^{1} \frac{zdz}{g_{\mathbf{p}}(z)} = x.$$

The next claim is [13, Theorem 1].[6]

▷ Claim B.2. $y_0(x) = \frac{1}{2}\left(1 - \mathfrak{h}_{\mathbf{p}}^2(x)\right)$.

Proof. Fix $x \in [0,1]$, let $\mathfrak{h} = \mathfrak{h}_{\mathbf{p}}(x)$ and $g(z) = g_{\mathbf{p}}(z)$. Define $\varphi : [0,\beta] \to [\mathfrak{h},1]$, where $\beta = y_1^{-1}(1-\mathfrak{h})$, as follows: $\varphi(u) = 1 - y_1(u)$. Note that by (8),

$$\varphi'(u) = -y_1'(u) = -\frac{g(\varphi(u))}{\varphi(u)}.$$

Thus

$$x = \int_{\mathfrak{h}}^{1} \frac{zdz}{g(z)} = -\int_{\varphi(0)}^{\varphi(\beta)} \frac{zdz}{g(z)} = -\int_{0}^{\beta} \frac{\varphi'(z)\varphi(z)dz}{g(\varphi(z))} = \beta,$$

hence $y_1(x) = 1 - \mathfrak{h}$. From (7) and (8) it follows that $y_0'(x) = g(\mathfrak{h}) = y_1'(x) \cdot \mathfrak{h} = -\mathfrak{h}\mathfrak{h}'$, and since $y_0(0) = 0$ it follows that $y_0(x) = \frac{1}{2}\left(1 - \mathfrak{h}^2\right)$. ◁

In particular, it follows from Claim B.2 that $\iota(\mathbb{T}_{\mathbf{p}}) = \frac{1}{2}\left(1 - \mathfrak{h}_{\mathbf{p}}^2(1)\right)$.

---

6 In [13] the authors required that the the degrees of the tree are all at least 2; we do not require this here.

C Proof of Theorem 6.4

1. It suffices to prove the claim for $v \in A$. First note that there exists a unique tree S_v in $T \star v$ which is not fully contained in A, and the rest of the trees are retained in the KC-transformation. The set of trees in $T' \star v$ which are not fully contained in A may be different from S_v, but they are on the same vertex set, so the result follows from subadditivity of α_n (Claim 6.1).
2. Write $|A| = a$, $|B| = b$ and $|P| = \ell + 1$. Let $A_1, \ldots, A_s$ be the trees of $T \star x$ which are fully contained in A, and denote $a_i = |A_i|$. Let $B_1, \ldots, B_t$ be the trees of $T \star y$ which are fully contained in B, and denote $b_i = |B_i|$. Let $\alpha_A = \sum_{i=1}^{s} \alpha_{a_i}$, $\alpha_A^+ = \sum_{i=1}^{s} \alpha_{1+a_i}$, $\alpha_B = \sum_{i=1}^{t} \alpha_{b_i}$ and $\alpha_B^+ = \sum_{i=1}^{t} \alpha_{1+b_i}$. Denote the vertices of P by $x = u_0, u_1, \ldots, u_\ell$. The following table summarises the values of ν in T, T' along vertices of P, in the case where $\ell \geq 3$ (similar tables can be made for the cases $\ell = 1, 2$).

	$\nu_{u_j}(T)$	$\nu_{u_j}(T')$
$j = 0$	$\alpha_A + \alpha_{b+\ell-1}$	$\alpha_A + \alpha_B + \alpha_{\ell-1}$
$j = 1$	$\alpha_A^+ + \alpha_{b+\ell-2}$	$\alpha_A^+ + \alpha_B^+ + \alpha_{\ell-2}$
$2 \leq j \leq \ell - 2$	$\alpha_{a+j-1} + \alpha_{b+\ell-j-1}$	$\alpha_{a+b+j-1} + \alpha_{\ell-j-1}$
$j = \ell - 1$	$\alpha_{a+\ell-2} + \alpha_B^+$	$\alpha_{a+b+\ell-2}$
$j = \ell$	$\alpha_{a+\ell-1} + \alpha_B$	$\alpha_{a+b+\ell-1}$

It follows (for every $\ell \geq 1$) that

$$\sum_{v \in P} (\nu_v(T') - \nu_v(T)) = \sum_{j=1}^{\ell-1} (\alpha_{a+b+j} + \alpha_j - \alpha_{a+j} - \alpha_{b+j})$$
$$= \xi_{a+b,\ell-1} + \xi_{0,\ell-1} - \xi_{a,\ell-1} - \xi_{b,\ell-1},$$

which is, by Claim 6.2, nonnegative. ◀

The Disordered Chinese Restaurant and Other Competing Growth Processes

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Abstract

The disordered Chinese restaurant process is a partition-valued stochastic process where the elements of the partitioned set are seen as customers sitting at different tables (the sets of the partition) in a restaurant. Each table is assigned a positive number called its attractiveness. At every step a customer enters the restaurant and either joins a table with a probability proportional to the product of its attractiveness and the number of customers sitting at the table, or occupies a previously unoccupied table, which is then assigned an attractiveness drawn from a bounded distribution independently of everything else. When all attractivenesses are equal to the upper bound this process is the classical Chinese restaurant process; we show that the introduction of disorder can drastically change the behaviour of the system. Our main results are distributional limit theorems for the scaled number of customers at the busiest table, and for the ratio of occupants at the busiest and second busiest table. The limiting distributions are universal, i.e. they do not depend on the distribution of the attractiveness. They follow from two general Poisson limit theorems for a broad class of processes consisting of families growing with different rates from different birth times, which have further applications, for example to preferential attachment networks.

2012 ACM Subject Classification Mathematics of computing → Stochastic processes

Keywords and phrases Chinese restaurant process, competing growth processes, reinforced branching processes, preferential attachment tree with fitness, Poisson processes

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.21

Related Version A full version of the paper is available at `https://arxiv.org/abs/1909.07690`.

Funding *Cécile Mailler*: EPSRC fellowship EP/R022186/1
Anna Senkevich: AS is supported by a scholarship from the EPSRC Centre for Doctoral Training in Statistical Applied Mathematics at Bath (SAMBa), under the project EP/L015684/1.

1 Introduction

In this paper we investigate properties of the largest family at a large but fixed time in a sequence of growing families that have different birth times and different exponential growth rates. The growth rates are given by a sequence $F_1, F_2, \ldots$ of bounded independent and identically distributed random variables, while the birth times $\tau_1, \tau_2, \ldots$ may be random and can depend in a general fashion on the growth processes. In the most interesting cases the birth times are themselves arising from an exponentially growing process so that the largest family at time t arises from a competition between the few families born early, which have more time to grow, and the many families born late, among which the occurrence of a higher birth rate is more probable. Our framework includes dynamic network models, where the families are nodes and their size is the degree, or a disordered version of the Chinese restaurant process, where the families are tables and their size is the number of occupants.

In the introduction, we illustrate and motivate our results in the context of the disordered Chinese restaurant process. In Sec. 2 we introduce our general framework and main result. Then, in Sec. 3, we show how our results apply to the Chinese restaurant process and a further example, the preferential attachment tree with fitness. Finally, in Sec. 4, we sketch the proofs of our main result and its corollary.

The disordered Chinese restaurant process

Fix a parameter $\theta \geq 0$ and a probability distribution μ on $(0,1)$. The disordered Chinese restaurant process is a Markov process $(Z^{(n)})_{n\geq 1}$ such that, for all $n \geq 1$, $Z^{(n)} = (Z_1^{(n)}, Z_2^{(n)}, \dots)$ is a sequence of integers satisfying that, for all $n \geq 1$,

- $\sum_{i=1}^{\infty} Z_i^{(n)} = n$,
- there exists k such that $Z_i^{(n)} = 0$ for all $i > k$ and $Z_i^{(n)} \geq 1$ for all $i \leq k$.

In particular

$$\bar{Z}^{(n)} := \left(\tfrac{1}{n} Z_1^{(n)}, \tfrac{1}{n} Z_2^{(n)}, \dots, \tfrac{1}{n} Z_k^{(n)}\right)$$

are the proportions of sets in the random partition, for every $n \in \mathbb{N}$. At time n, the vector $Z^{(n)}$ can be interpreted as describing the distribution of n customers sitting at different (ordered) tables in a restaurant; for all $i \geq 1$, $Z_i^{(n)}$ is the number of customers sitting at the i-th table at time n. The distribution of the process is defined as follows: we sample a sequence $(F_i)_{i\geq 1}$ of i.i.d. random variables (the attractivenesses or fitnesses) from the distribution μ. We set $Z^{(1)} = (1, 0, 0, \dots)$ and, for all $n \geq 1$, given $Z^{(n)}$, we define $Z^{(n+1)}$ as follows: A new customer enters the restaurant, and

- with probability $F_i Z_i^{(n)}/(n+\theta)$ the new customer sits at the i-th table, i.e. we set $Z_j^{(n+1)} = Z_j^{(n)} + \mathbf{1}_{j=i}$ for all $1 \leq j \leq n$;
- otherwise, i.e. with the remaining probability

  $$1 - \frac{\sum_{i=1}^{\infty} F_i Z_i^{(n)}}{n+\theta},$$

  the new customer sits at table $k+1 := \min\{i \geq 1 \colon Z_i^{(n)} \neq 0\}$, i.e. we set $Z_{k+1}^{(n+1)} = 1$ and $Z_i^{(n+1)} = Z_i^{(n)}$ for all $1 \leq i \leq k$.

Taking $\mu = \delta_1$ (i.e. all fitnesses equal to one) gives the original Chinese restaurant process of Pitman, sometimes also called *temporal Dirichlet process* in the context of community detection algorithms (see e.g. [10]). In this case the sequence $(\bar{Z}^{(n)})$ with entries arranged in decreasing order converges in distribution to the Poisson-Dirichlet distribution of parameter θ. A corollary of our main result is that, under mild assumptions on μ, the proportion of customers sitting at the largest table in the disordered Chinese restaurant process vanishes asymptotically. In fact, we prove convergence of the properly-rescaled size of the busiest table to a Fréchet distribution. We state our precise assumptions on the distribution μ before stating our limiting theorems for the disordered Chinese restaurant process.

Assumptions on the fitness distribution

The behaviour of $(Z^{(n)})_{n\geq 1}$ depends on the fitness distribution μ. In this paper, we assume that μ is supported by a bounded interval, which we may take as $(0,1)$. We are interested in the largest tables in the disordered Chinese restaurant process, and fitter tables are more likely to get larger; therefore, records in the sequence of random fitnesses play an important role. These records are governed by the fitness distribution μ, more precisely by its tail near 1, and extreme value theory gives information about their behaviour.

The Fisher–Tippett–Gnedenko theorem of extreme value theory says that, if there exist two sequences $(\alpha_n)_{n\geq 1}$, $(\beta_n)_{n\geq 1}$ and a probability distribution Υ such that

$$\frac{\max_{1\leq i\leq n} F_i - \beta_n}{\alpha_n} \to \Upsilon,$$

then Υ is either the Gumbel or the Weibull distribution (for unbounded random variabes it can be either Gumbel or Fréchet). Intuitively, the Gumbel distribution corresponds to fitness distributions μ with light, and the Weibull distribution to fitness distributions with heavy tail near 1. In this paper, we therefore distinguish between (A) distributions μ that are in the maximum domain of attraction of a Gumbel distribution and (B) distributions that are in the maximum domain of attraction of a Weibull distribution.

More precisely, we assume one of the following:

- **(A0)** The function $m(x) = -\log \mu((x, 1))$ is twice differentiable and satisfies
  - **(A0.1)** $m'(x) > 0$ and $m''(x) > 0$ for all $x \in (0, 1)$;
  - **(A0.2)** $\lim_{x\uparrow 1} \frac{m''(x)}{(m'(x))^2} = 0$;
  - **(A0.3)** $\exists \varkappa > 0$ such that $\lim_{x\uparrow 1} \frac{m''(x)m(x)x}{(m'(x))^2} = \varkappa$;
  - **(A0.4)** $\lim_{x\uparrow 1} \frac{m(x)}{m'(x)} = 0$.
- **(B0)** The fitness distribution μ has a regularly varying tail in one, meaning that there exists $\alpha > 1$ and a slowly varying function ℓ with $\mu((1-\varepsilon, 1)) = \varepsilon^\alpha \ell(\varepsilon)$.

▶ Note 1. A typical example of probability distribution satisfying **(A0)** is $\mu((x, 1)) = \exp\left(1 - (1-x)^{-\rho}\right)$ for all $x \in (0, 1)$, $\rho > 0$. Heuristically, **(A0)** asks for a lighter tail near the essential supremum than **(B0)**.

▶ Note 2. Assumptions **(A0-i)** and **(A0-ii)** imply that the fitness distribution μ lies in the maximum domain of attraction of the Gumbel distribution. Although most of the natural examples satisfy Assumptions **(A0-iii)** and **(A0-iv)**, some probability distributions in the maximum domain of attraction of the Gumbel distribution do not fall into our framework. One example is $m(x) = \log\left(\frac{\mathrm{e}}{1-x}\right) \log\log\left(\frac{\mathrm{e}}{1-x}\right)$ (see [9, 8] for details).

Limiting theorems for the disordered Chinese restaurant process

We first state a result on the number of tables occupied after n steps.

▶ **Proposition 3.** *The number K_n of occupied tables when there are n customers satisfies*

$$\lim_{n\to\infty} \frac{K_n}{n} = \left(\int \frac{\mu(\mathrm{d}x)}{1-x}\right)^{-1} \quad \textit{almost surely.}$$

This result is in contrast to the classical Chinese restaurant process where the number of tables grows only logarithmically. The next two propositions follow from our main result, which we state in Section 2 in the much more general context of *competing growth processes*.

First, we look at the rescaled occupancy of the largest table. Other than in the classical Chinese restaurant process the occupancy of tables turns out not to be macroscopic and the proportions $(\bar{Z}^{(n)})$ do not converge to a limiting partition. This is not surprising, as the probability of the n-th customer starting a new table is of constant order in this case but of order $1/n$ in the classical case.

▶ **Proposition 4.** *If μ satisfies either **(A0)** or **(B0)**, then the number of occupants at the largest table satisfies*

$$\lim_{n\to\infty} \frac{1}{n}\big(\max_{i\geq 1} Z_i^{(n)}\big) = 0 \qquad \textit{almost surely.}$$

*Under Assumption **(B0)**, we further have that, in distribution when $n \to \infty$,*

$$\frac{(\log n)^\alpha}{n\ell(\frac{1}{\log n})}\big(\max_{i\geq 1} Z_i^{(n)}\big) \Rightarrow W,$$

where W is a standard Fréchet distribution.

▶ Note 5. In the context of our main result we also provide a limit theorem under assumption **(A0)**, which reveals the universal nature of the limiting Fréchet distribution, see Corollary 12.

Second, we look at the ratio of the sizes of the two busiest tables and again see universal behaviour, irrespective of whether μ is from the maximum domain of attraction of the Gumbel or Weibull distribution.

▶ **Proposition 6.** *For all integers n, we denote by $R_n \geq 1$ the ratio of the sizes of the largest and second largest tables at time n. If μ satisfies **(A0)** or **(B0)**, then*

$$\lim_{n\to\infty} \mathbb{P}(R_n \geq x) = {}^1\!/\!_x \qquad \textit{for all } x \geq 1.$$

2 General framework and main result

We now describe our general framework (in a slightly less general version than in [5]), which is a continuous time process defined as follows: Given μ a probability distribution on $(0,1)$, let

- $(F_n)_{n\geq 1}$ be a sequence of i.i.d. μ-distributed random variables;
- $(\tau_n)_{n\geq 1}$ be a non-decreasing sequence of positive random variables with $\tau_1 = 0$;
- for all $n \geq 1$ and $t \geq \tau_n$, $Z_n(t) = Y_n(F_n(t-\tau_n))$ for a family $(Y_n(t) : t \geq 0)_{n\geq 1}$ of i.i.d. non-decreasing integer-valued processes independent of $(F_n)_{n\geq 1}$.

Define $M(t) := \max\{n : \tau_n \leq t\}$ and $N(t) := \sum_{n=1}^{M(t)} Z_n(t)$. We view this as a population of immortal individuals and we refer to $Z_n(t)$ as the size of the n-th family, $M(t)$ the number of families in the system and $N(t)$ the total size of the population respectively, at time t. From this perspective τ_n represents the foundation time of the n-th family. We see F_n as a fitness parameter of the n-th family, determining the rate at which new offsprings are born into it.

In this paper we aim at proving convergence results for the maximal family in the population. For this we require the following assumptions **(A1), (A3), (A4)** on the growth processes, in addition to Assumption **(A0)** or **(B0)** on the fitness distribution (a condition called **(A2)** is only needed in the more general setup of [5]).

Assumptions

- **(A1) Families' foundation times:** There exists $\lambda > 0$ such that, for all $n \in \mathbb{N}$,

  $$\tau_n = \tau_n^* + T + \varepsilon_n,$$

  where $\tau_n^* := \frac{1}{\lambda}\log n$, T is a finite random variable, and $\varepsilon_n \to 0$ almost surely as $n \to \infty$.

- **(A3) Growth rate:** There exists $\gamma > 0$ and an integrable random variable ξ with density ν defined on $[0, \infty)$, such that

$$\mathrm{e}^{-\gamma t} Y_1(t) \longrightarrow \xi, \qquad \text{almost surely as } t \to \infty.$$

- **(A4) Concentration of growth:** There exist $c_0, \eta > 0$ such that

$$\mathbb{P}\big(\max_{u \geq 0} Y_1(u)\mathrm{e}^{-\gamma u} \geq x\big) \leq c_0 \mathrm{e}^{-\eta x}, \qquad \text{for all } x \geq 0.$$

▶ Note 7. These three assumptions all have the same aim: our results rely on controlling the growth rates of the population and of each of the families. Assumption (A1) gives some control over the growth of the process in terms of numbers of families; λ can be interpreted as the "Malthusian" parameter of the process (see, e.g. [6], where the concept of Malthusian growth is studied in the context of Crump-Mode-Jagers processes). Assumptions (A3) and (A4) gives some control over the growth of each of the families.

To state our main result, we need to define σ_t, which approximates the birth time of the family that is the largest at time t.

- Under Assumption **(A0)** on μ, we define σ_t as the unique solution of

$$(\log g)'(\lambda \sigma_t) = \frac{1}{\lambda(t - \sigma_t)}, \tag{1}$$

  where $g(x) = m^{-1}(x)$, see [5, Lemma 5] for a proof of existence and uniqueness of σ_t.
- Under Assumption **(B0)** on μ, we set $\sigma_t := \tau_{n(t)}$, where $n(t) = \lceil \mu(1 - t^{-1}, 1)^{-1} \rceil$. Then $\log n(t) \sim \alpha \log t - \log \ell(1/t)$ and Assumption **(A1)** implies that

$$\sigma_t = \frac{1}{\lambda} \log n(t) + T + o(1) = \frac{\alpha}{\lambda} \log t - \frac{1}{\lambda} \log \ell(1/t) + T + o(1) \tag{2}$$

Main result under Assumption (B0)

We now state our results, first in the easier case of μ satisfying Assumption **(B0)**. For all $t \geq 0$, we define the point process

$$\Gamma_t = \sum_{n=1}^{M(t)} \delta\big(\tau_n - \sigma_t, t(1 - F_n), \mathrm{e}^{-\gamma(t - \sigma_t)} Z_n(t)\big), \tag{3}$$

on $(-\infty, \infty) \times (0, \infty) \times (0, \infty)$, where $\delta(x)$ is the Dirac mass at x.

▶ **Theorem 8** (Poisson limit). *Under Assumptions **(B0)** and **(A1)**, **(A3)**, **(A4)**, the point process $(\Gamma_t)_{t \geq 0}$ converges vaguely*[1] *on the space $[-\infty, \infty] \times [0, \infty] \times (0, \infty]$ to the Poisson point process with intensity measure*

$$\mathrm{d}\zeta(s, f, z) = \alpha f^{\alpha - 1} \lambda \mathrm{e}^{\lambda s} \mathrm{e}^{\gamma(s + f)} \nu(z \mathrm{e}^{\gamma(s + f)})\, \mathrm{d}s\, \mathrm{d}f\, \mathrm{d}z,$$

*where ν is defined in **(A3)**.*

Observe that the compactification of the intervals in Theorem 8 ensures that the point with the largest z-component in the Poisson point process corresponds asymptotically to the family of maximal size. Theorem 8 therefore implies the following distributional limit.

---

[1] We say that a sequence of measures $(\mu_n)_{n \in \mathbb{N}}$ on a topological space $\mathbb{X}$ converges *vaguely* to μ iff $\int f \mathrm{d}\mu_n \to \int f \mathrm{d}\mu$, as $n \to \infty$, for all continuous functions $f \colon \mathbb{X} \to \mathbb{R}$ with compact support.

▶ **Corollary 9.** *Let $V(t)$ be the fitness of the family of maximal size at time t. Then,*

$$t(1 - V(t)) \Rightarrow V \qquad \text{as } t \to \infty,$$

where V is Gamma distributed with shape parameter α and scale parameter λ.

Theorem 8 and Corollary 9 are proved in [9]. The proofs are based on similar ideas as the proofs outlined here, but the execution of these ideas is much simpler. A similar result in a different, less general setup can be found in [3].

Main result under Assumption (A0)

To now state *our main results* we look at fitness distributions satisfying Assumption **(A0)**. For all $t \geq 0$, we define

$$\Gamma_t = \sum_{n=1}^{M(t)} \delta\Big(\frac{\tau_n - \sigma_t}{\sqrt{\sigma_t}}, \frac{F_n - g\big(\log(n\sqrt{\sigma_t})\big)}{g'\big(\log(n\sqrt{\sigma_t})\big)}, \mathrm{e}^{-\gamma g(\lambda\sigma_t)(t-\sigma_t) - a_1 g(\lambda\sigma_t)\log\sigma_t + \gamma T} Z_n(t)\Big), \tag{4}$$

where $\delta(x)$ is the Dirac mass at x, and $a_1 := \frac{\gamma}{2\lambda}$.

▶ **Theorem 10** (Poisson limit). *Under Assumptions **(A0)**, **(A1)**, **(A3)**, **(A4)**, the point process $(\Gamma_t)_{t\geq 0}$ converges vaguely on the space $[-\infty, \infty] \times [-\infty, \infty] \times (0, \infty]$ to the Poisson point process with intensity measure*

$$\mathrm{d}\zeta(s,\, f,\, z) = \lambda \mathrm{e}^{-f} \mathrm{e}^{s^2 a_2 - f a_3} \nu(z \mathrm{e}^{s^2 a_2 - f a_3})\, \mathrm{d}s\, \mathrm{d}f\, \mathrm{d}z,$$

*where $a_2 := \frac{\gamma}{2}\varkappa$, $a_3 := \frac{\gamma}{\lambda}$ and ν is as in **(A3)**.*

▶ Note 11. The existence of a density for the random variable ξ is assumed in Assumption **(A3)** for convenience only. For example, Theorem 8 and 10 continue to hold if $\nu = \delta_1$.

The technical difference between Theorems 8 and 10 is that in the latter the first (birthtime) coordinate needs to be scaled. As a result the scaling of the second (fitness) component depends on the birth rank n of the family as well as on the observation time t. Therefore we cannot derive a general scaling limit for the fitness of the largest family as in Corollary 9. However, results for the size of this family are still possible and allow an interesting comparison.

▶ **Corollary 12.**

(i) *Under Assumption **(B0)**, asymptotically as $t \to \infty$,*

$$\mathrm{e}^{-\gamma t + \frac{\gamma\alpha}{\lambda}\log t - \frac{\gamma}{\lambda}\log \ell(1/t) + \gamma T} \max_{n\in\mathbb{N}} Z_n(t) \Rightarrow W,$$

where W is Fréchet-distributed with shape parameter λ/γ and scale parameter s, where

$$s^{\frac{\lambda}{\gamma}} = \Gamma(\alpha+1)\lambda^{-\alpha} \int_0^\infty \nu(w) w^{\frac{\lambda}{\gamma}}\, \mathrm{d}w.$$

(ii) *Under Assumption **(A0)**, asymptotically as $t \to \infty$,*

$$\mathrm{e}^{-\gamma g(\lambda\sigma_t)(t-\sigma_t) - a_1 g(\lambda\sigma_t)\log\sigma_t + \gamma T} \max_{n\in\mathbb{N}} Z_n(t) \Rightarrow W,$$

where W is Fréchet-distributed with shape parameter λ/γ and scale parameter s, where

$$s^{\frac{\lambda}{\gamma}} = \sqrt{\tfrac{2\pi\lambda}{\varkappa}} \int_0^\infty \nu(w) w^{\frac{\lambda}{\gamma}}\, \mathrm{d}w.$$

▶ Note 13. Observe that irrespective of whether μ is in the maximum domain of attraction of the Weibull or Gumbel distribution, the size of the largest family scaled by a deterministic function of time and the random factor $\mathrm{e}^{\gamma T}$ converges to a Fréchet distribution.

3 Applications of our main results

Embedding the disordered Chinese restaurant process

The key to the application of our main result to a discrete process such as the disordered Chinese restaurant process is a clever choice of embedding into continuous time. Customers now enter the restaurant at some random times $0 =: T_0 < T_1 < T_2, \dots$ defined inductively as follows. At time T_n we start $n+1$ independent exponential clocks, one clock of parameter one for each of the n customers seated in the restaurant and one additional clock of parameter θ for the creation of an additional table. We let T_{n+1} be the time when the first of these clocks rings.

- If it is the clock corresponding to customer m sitting at table j we toss a coin with success probability F_j.
  - If there is a success the $(n+1)$-th customer joins this table,
  - if there is no success the $(n+1)$-th customer seats at a new table which, if it is the $(k+1)$-th occupied table, gets fitness F_{k+1}.
- If it is the clock for the creation of additional tables, the $(n+1)$-th customer also sits at a new table which, if it is the $(k+1)$-th occupied table, gets fitness F_{k+1}.

Suppose $F_1, F_2, \dots$ are given. We note that, as required, the overall probability that a new table is created at time T_{n+1} is

$$\frac{\sum_{j=1}^{k} Z_j(T_n)(1-F_j)+\theta}{n+\theta} = 1 - \frac{\sum_{j=1}^{k} Z_j(T_n)F_j}{n+\theta},$$

where $Z_j(T_n)$ is the number of occupants at the j-th table at time T_n, and the probability that the $(n+1)$-th customer joins the j-th table is $Z_j(T_n)F_j/(n+\theta)$. Therefore this continuous-time processes taken at the successive times $T_0, T_1, \dots$ is equal in distribution to the disordered Chinese restaurant process defined in Section 1, as required.

Looking at the j-th table, we let τ_j be the time when it is first occupied. If at time t this table is occupied by m customers the rate at which new customers join this table is mF_j, independently of the occupancy of other tables. The processes $(Z_j(t+\tau_j) \colon t \geq 0)$ are therefore independent Yule processes with rate F_j. Hence Assumptions **(A3), (A4)** are satisfied for $\gamma = 1$. To check Assumption **(A1)** we note that the process of introduction of new tables is a general branching process with immigration. The immigration process corresponds to the creation of the additional tables, which is a homogeneous Poisson process with rate θ. The point process of creation of tables by unsuccessful coin tossing is a Cox process $(\Pi(t) \colon t \geq 0)$, i.e. a Poisson process with random intensity. Its intensity is given by $(1-F)Y(t)\,\mathrm{d}t$ where F has distribution μ and given F the process $(Y(t) \colon t \geq 0)$ is a Yule process with parameter F. The relevant results for general branching processes can be found in [6] with the case of branching processes with immigration treated in [7]. The crucial assumption is the existence of a Malthuisan parameter $\alpha \geq 0$ such that

$$1 = \int \mathrm{e}^{-\alpha t}\, \mathbb{E}\Pi(\mathrm{d}t) = \int \int_0^\infty (1-w)\mathrm{e}^{-\alpha t} e^{wt}\, dt\, \mu(\mathrm{d}w) = \int \frac{1-w}{\alpha - w}\, \mu(\mathrm{d}w),$$

which is always satisfied for $\alpha = 1$. Under an additional $x \log x$ condition on $\int \mathrm{e}^{-t}\Pi(\mathrm{d}t)$, which can be checked by straightforward but long calculations, we get from [6, Theorem 5.4] for general branching processes without immigration (our case $\theta = 0$) and modifications described in [7, Theorem 4.2] for the general case (stated there only for convergence in L^1) that there exists a positive random variable N_θ such that the total nnumber $M(t)$ of tables occupied by time t satisfies

$$\mathrm{e}^{-t} M(t) \longrightarrow N_\theta \quad \text{almost surely,}$$

from which we infer that $\tau_n = \log n - \log N_\theta + o(1)$, implying that **(A1)** holds with $\lambda = 1$.

Disordered Chinese restaurant process – proof of Proposition 3

We first find the limit of the empirical fitness distributions. This can be accomplished using the stochastic approximation technique of Dereich and Ortgiese [4] and does not require continuous time embedding. Suppose for illustration that μ has finite support $\{f_1, \dots, f_m\}$ and let $X_n(i)$ be the proportion of customers sitting at a table with attractiveness f_i and $(\mathfrak{G}_n)_{n\geq 1}$ be the natural filtration. Then we have the equality

$$\mathbb{E}\big[X_{n+1}(i) - X_n(i) \big| \mathfrak{G}_n\big] = \frac{1}{n+1}\Big(\mu(\{f_i\})\Big[1 - \frac{n}{n+\theta}\bar{F}_n\Big] + \frac{n f_i}{n+\theta} X_n(i) - X_n(i)\Big),$$

where $\bar{F}_n = \sum_{j=1}^m f_j X_n(j) = \frac{1}{n}\sum_{i=1}^{K_n} F_i Z_i^{(n)}$. Using stochastic approximation techniques developed by [4] (these techniques also work without our illustrative assumption), one can show that if $\limsup \bar{F}_n \leq \eta$ (resp. $\liminf \bar{F}_n \geq \eta$), then for all $0 \leq a \leq b \leq 1$,

$$\liminf \frac{1}{n}\sum_{i=1}^{K_n} \mathbf{1}_{F_i \in (a,b]} Z_i^{(n)} \geq \int_a^b \frac{1-\eta}{1-x}\,\mu(\mathrm{d}x) \tag{5}$$

$$\Big(\text{resp. } \limsup \frac{1}{n}\sum_{i=1}^{K_n} \mathbf{1}_{F_i \in (a,b]} Z_i^{(n)} \leq \int_a^b \frac{1-\eta}{1-x}\,\mu(\mathrm{d}x)\Big).$$

Iterating, e.g. the upper bound, we get

$$\limsup \bar{F}_n \leq (1-\eta)\int \frac{x}{1-x}\,\mu(\mathrm{d}x) =: T(\eta),$$

and eventually convergence of $(\bar{F}_n)$ to the fixed point $\eta^* \in (0,1)$ of T, which is

$$\eta^* = 1 - \Big(\int \frac{\mu(\mathrm{d}x)}{1-x}\Big)^{-1}.$$

Together with Equation (5), this implies that, for all $0 \leq a \leq b \leq 1$,

$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{K_n} \mathbf{1}_{F_i \in (a,b]} Z_i^{(n)} = \int_a^b \frac{1-\eta^*}{1-x}\mu(\mathrm{d}x) \quad \text{almost surely.}$$

By construction, the conditional probability that a newly arriving customer establishes a new table is therefore converging to

$$\int (1-x)\frac{1-\eta^*}{1-x}\mu(\mathrm{d}x) = \Big(\int \frac{\mu(\mathrm{d}x)}{1-x}\Big)^{-1},$$

which is also the asymptotic ratio of tables per customer, as claimed.

Disordered Chinese restaurant process – proof of Proposition 4

This follows from Corollary 12 (recall that in this case $\lambda = \gamma = 1$). In both parts, plugging $t = \tau_n$ shows that the leading term in the scaling is $\frac{1}{n}$ and all further factors together go to infinity. Under Assumption **(B0)**, we get that

$$\begin{aligned}&\exp(-\tau_n + \alpha \log \tau_n - \log \ell(1/\tau_n) + T)\\ &\quad= \exp\big(-\log n - T - \log \ell(\tfrac{1}{\log n}) + \alpha \log\log n + T + o(1)\big) = \frac{(\log n)^\alpha}{n\ell(\frac{1}{\log n})}(1+o(1)),\end{aligned}$$

and thus, by Corollary 12**(i)**, $(\log n)^\alpha \max Z_i^{(n)}/(n\ell(\frac{1}{\log n}))$ converges in distribution to a Fréchet as claimed. Under Assumption **(A0)**, we have that, asymptotically when $t \uparrow \infty$,

$$-g(\sigma_t)(t-\sigma_t) - g(\sigma_t)\log \sigma_t = -t + \sigma_t + h(\sigma_t)t + o(\sigma_t) + o(h(\sigma_t)t),$$

where $h(x) = 1 - g(x) \downarrow 0$ when $x \uparrow \infty$. Taking $t = \tau_n = \log n + T + \varepsilon_n$ thus gives $\mathrm{e}^{u_n} \max Z_i^{(n)}/n \Rightarrow W$, where $u_n = (\sigma_{\tau_n} + h(\sigma_{\tau_n})\tau_n)(1+o(1)) \uparrow \infty$, which concludes the proof.

Disordered Chinese restaurant process – proof of Proposition 6

We denote by $R(t)$ the ratio of the sizes of the largest and second largest tables (i.e. families in the competing growth process) at time t. Let us first assume that μ satisfies Assumption **(A0)**. By Theorem 10, we have, for all $x > 1$,

$$\lim_{t\to\infty} \mathbb{P}\big(R(t) \geq x\big) = \iiint \exp\big(-\zeta\big((-\infty,\infty)\times(-\infty,\infty)\times(z/x,\infty)\big)\big)\,\zeta(\mathrm{d}s\,\mathrm{d}f\,\mathrm{d}z).$$

Using that $\nu(x) = \mathrm{e}^{-x}$ and $a_3 = 1$ in the first equality and the change of variable $v = f - \log y$ in the second, we get that

$$\begin{aligned}\zeta\big((-\infty,\infty)\times(-\infty,\infty)\times(z/x,\infty)\big) &= \iint \mathrm{d}s\,\mathrm{d}f\,\mathrm{e}^{s^2a_2-2f}\int_{z/x}^\infty \mathrm{e}^{-y\mathrm{e}^{s^2a_2-f}}\,\mathrm{d}y\\ &= \iint \mathrm{d}s\,\mathrm{d}v\,\mathrm{e}^{s^2a_2-2v}\mathrm{e}^{-\mathrm{e}^{s^2a_2-v}}\int_{z/x}^\infty y^{-2}\,\mathrm{d}y = a_5\,\frac{x}{z},\end{aligned}$$

where a_5 is a positive constant. Hence, substituting f by $f + \log x$ in the final step,

$$\begin{aligned}\lim_{t\to\infty} \mathbb{P}\big(R(t) \geq x\big) &= \iint \mathrm{d}s\,\mathrm{d}f \int_0^\infty \mathrm{d}z\,\mathrm{e}^{-f}\mathrm{e}^{s^2a_2-f}\mathrm{e}^{-z(\mathrm{e}^{s^2a_2-f})-a_5\frac{x}{z}}\\ &= \iint \mathrm{d}s\,\mathrm{d}f\int_0^\infty \mathrm{d}w\,\mathrm{e}^{-f}\mathrm{e}^{-w-a_5\frac{1}{w}\mathrm{e}^{s^2a_2-f+\log x}} = \frac{1}{x}.\end{aligned}$$

Similarly, if μ satisfies Assumptions **(B0)**, we have $\zeta\big((-\infty,\infty)\times(0,\infty)\times(z/x,\infty)\big) = a_6\,\frac{x}{z}$, and hence by Theorem 8 (and using the change of variable $z \to z/x$ in the second equality),

$$\begin{aligned}\lim_{t\to\infty} \mathbb{P}\big(R(t) \geq x\big) &= \int \mathrm{d}s \int_0^\infty \mathrm{d}f \int_0^\infty \mathrm{d}z\,\alpha f^{\alpha-1}\mathrm{e}^{2s+f}\mathrm{e}^{-z\mathrm{e}^{s+f}-a_6\frac{x}{z}}\\ &= \int \mathrm{d}s \int_0^\infty \mathrm{d}f \int_0^\infty \mathrm{d}z\,x\,\alpha f^{\alpha-1}\mathrm{e}^{2s+f}\mathrm{e}^{-z\mathrm{e}^{s+f+\log x}-a_6\frac{1}{z}} = \frac{1}{x},\end{aligned}$$

substituting s by $s + \log x$ in the final step. This concludes the proof of Proposition 6.

Preferential attachment networks with fitness

In this subsection, we show how our results can be used to get asymptotic information about the node of largest degree in preferential attachment networks with fitness. We focus on the Bianconi-Barabási model, first introduced by Bianconi and Barabási in [1], but one can also find an application of our main results to the model of Dereich [2] in [5, Sec. 2.2.2]. In the Bianconi and Barabási model, nodes join a network one by one and create a link with an existing node chosen at random with probability proportional to its degree in the network times its *fitness*. The process starts with two vertices connected by an edge. The fitness of each node is a positive number sampled according to a distribution μ, independently from the rest of the process. Although generalisations exists, we only treat the tree-version of this model: each node creates only one extra edge when joining the network. We show that under a Malthusian condition the continuous-time embedding of the Bianconi and Barabási tree is a competing growth process and that our main results apply to this model.

In this embedding, τ_n is the birthtime of the n-th vertex, F_n its fitness and $Z_n(t)$ its degree at time t. One can show (see [5, Sec. 5.1]) that under the Malthusian condition

$$\int_0^1 \frac{\mu(\mathrm{d}x)}{1-x} > 2,$$

the process satisfies **(A1)**, **(A3)**, **(A4)** with $\gamma = 1$ and $\lambda > 1$ the unique solution of

$$\int_0^1 \frac{x}{\lambda - x}\,\mu(\mathrm{d}x) = 1.$$

Our main results thus apply and give, for example, precise asymptotic estimates for the largest degree in the network.

▶ **Proposition 14.** *Assume that there exists $\varrho \in (0,1)$ such that, for all $x \in (0,1)$, $\mu((x,1)) = \exp(1-(1-x)^{-\varrho})$. Denote by D_n the largest degree in the Bianconi and Barabási tree with n vertices. Then, as $n \to \infty$, we have, in probability,*

$$D_n = \exp\Big(\frac{1}{\lambda}\log n - \frac{a_4}{\lambda}(\log n)^{\frac{\varrho}{\varrho+1}} - \frac{a_5}{\lambda}\log\log n + \mathcal{O}(1)\Big),$$

where $a_4 = \varrho^{-\frac{\varrho}{\varrho+1}} + \varrho^{\frac{1}{\varrho+1}}$ and $a_5 = \frac{\varrho}{2(\varrho+1)}$.

Proof. First recall that this fitness distribution satisfies Assumption **(A0)**, and thus Theorem 10 and Corollary 12**(ii)** apply. We estimate σ_t as defined in Equation (1). Since $g(x) = m^{-1}(x) = 1-(x+1)^{-1/\varrho}$, we have that $x = \lambda\sigma_t$ is the unique solution of

$$(\log g)'(x) = \frac{1}{\lambda t + 1 - (x+1)} = \frac{1}{\varrho(x+1)^{\frac{\varrho+1}{\varrho}} - \varrho(x+1)},$$

which implies $\sigma_t = \lambda^{-\frac{1}{\varrho+1}}(t/\varrho)^{\frac{\varrho}{\varrho+1}} + \mathcal{O}\big(t^{\frac{\varrho-1}{\varrho+1}}\big)$. By definition of $\varkappa$ in Assumption **(B0)** we get

$$\varkappa = \lim_{x\uparrow 1}\frac{m''(x)m(x)x}{(m'(x))^2} = \lim_{x\uparrow 1}\frac{(\varrho+1)x\big(1-(1-x)^{\varrho}\big)}{\varrho} = \frac{\varrho+1}{\varrho}.$$

By Corollary 10**(ii)**, we get that, asymptotically when $t \to \infty$,

$$\mathrm{e}^{-\left(t - a_4\lambda^{-\frac{1}{1+\varrho}}t^{\frac{\varrho}{\varrho+1}} + \frac{1}{\lambda}\right) - \frac{1}{\lambda}a_5\log t + T}\max_{n\in\mathbb{N}} Z_n(t) \Rightarrow W,$$

where W is a Fréchet-distributed random variable with shape parameter λ and scale parameter s given by $s^\lambda = \sqrt{\frac{2\pi\varrho}{\varrho+1}}\Gamma(\lambda+1)$. To get a result for discrete-time process we need to estimate the time τ_n when the $(n+1)$-th vertex is introduced to the network. By Assumption **(A1)**, we know that $\tau_n = \frac{1}{\lambda}\log n + T + \varepsilon_n$, which concludes the proof. ◀

4 Sketch of the proofs

We give sketches of the proofs in the case of Assumption **(A0)**; the proofs under Assumption **(B0)** are similar but easier (these proofs are detailed in [9, Ch. 3]).

Sketch of the proof of Corollary 12(ii)

We fix $x > 0$ and $B := [-\infty, \infty] \times [-\infty, \infty] \times [x, \infty]$. By Theorem 10, we get that, as $t \uparrow \infty$,

$$\sum_{n=1}^{M(t)} \mathbf{1}_B\Big(\tfrac{\tau_n - \sigma_t}{\sqrt{\sigma_t}}, \tfrac{F_n - g(\log(n\sqrt{\sigma_t}))}{g'(\log(n\sqrt{\sigma_t}))}, \mathrm{e}^{-\gamma g(\lambda\sigma_t)(t-\sigma_t) - a_1 g(\lambda\sigma_t)\log\sigma_t + \gamma T} Z_n(t)\Big) \Rightarrow \mathrm{Poisson}\Big(\int_B \mathrm{d}\zeta\Big),$$

since B is a compact set. Hence, as $t \uparrow \infty$,

$$\begin{aligned}&\mathbb{P}\Big(\mathrm{e}^{-\gamma g(\lambda\sigma_t)(t-\sigma_t) - a_1 g(\lambda\sigma_t)\log\sigma_t + \gamma T} \max_{n\in\{1,\dots,M(t)\}} Z_n(t) \geq x\Big) \\ &\quad \to \mathbb{P}\Big(\mathrm{Poisson}\Big(\int_B \mathrm{d}\zeta\Big) \geq 1\Big) = 1 - \mathbb{P}\Big(\mathrm{Poisson}\Big(\int_B \mathrm{d}\zeta\Big) = 0\Big) = 1 - \exp\Big(-\int_B \mathrm{d}\zeta\Big).\end{aligned} \tag{6}$$

One can check that

$$\int_B \mathrm{d}\zeta = \lambda\sqrt{\pi\frac{a_3}{a_2}}\Big(\int_0^\infty \nu(w) w^{\frac{1}{a_3}}\,\mathrm{d}w\Big) x^{-\frac{1}{a_3}}. \tag{7}$$

Recall that $a_2 = \gamma\varkappa/2$ and $a_3 = \gamma/\lambda$. Thus the right hand side in (6) is $1 - \exp(-s^\eta x^{-\eta})$, for

$$s^\eta = \sqrt{\tfrac{2\pi\lambda}{\varkappa}} \int_0^\infty \nu(w) w^{\frac{\lambda}{\gamma}}\,\mathrm{d}w, \quad \text{and } \eta = \frac{\lambda}{\gamma}.$$

In summary, for all $x > 0$, we have

$$\mathbb{P}\Big(\mathrm{e}^{-\gamma g(\lambda\sigma_t)(t-\sigma_t) - a_1 g(\lambda\sigma_t)\log\sigma_t + \gamma T} \max_{n\in\{1,\dots,M(t)\}} Z_n(t) \leq x\Big) \quad \to \quad \mathrm{e}^{-(x/s)^{-\frac{\lambda}{\gamma}}} = \mathbb{P}(W \leq x),$$

where $W \sim$ Fréchet $\big(\frac{\lambda}{\gamma}, s\big)$, which concludes the proof.

Sketch of the proof of Theorem 10 (for details see [5, Sec. 4])

The idea of the proof is to first give convergence of the point process on the domain $(-\infty, \infty) \times (-\infty, \infty) \times [0, \infty]$ and second get the "right" shapes of the brackets by showing that all the families that are born either too early or too late, or have a fitness that is too small have a renormalised size that goes to zero. First we prove the following result, which we sketch-proof in the next paragraph:

▶ **Proposition 15.** *The point process*

$$\Gamma_t = \sum_{n=1}^{M(t)} \delta\Big(\frac{\tau_n - \sigma_t}{\sqrt{\sigma_t}}, \frac{F_n - g\big(\log(n\sqrt{\sigma_t})\big)}{g'\big(\log(n\sqrt{\sigma_t})\big)}, \mathrm{e}^{-\gamma g(\lambda\sigma_t)(t-\sigma_t) - a_1 g(\lambda\sigma_t)\log\sigma_t + \gamma T} Z_n(t)\Big),$$

converges vaguely in distribution on $(-\infty, \infty) \times (-\infty, \infty) \times [0, \infty]$ to the Poisson point process with intensity

$$\zeta(\mathrm{d}s,\, \mathrm{d}f,\, \mathrm{d}z) = \lambda \mathrm{e}^{-f} \mathrm{e}^{s^2 a_2 - f a_3} \nu(z \mathrm{e}^{s^2 a_2 - f a_3})\,\mathrm{d}s\,\mathrm{d}f\,\mathrm{d}z.$$

The main difference between Proposition 15 and Theorem 10 is the shape of the brackets in the domain of convergence. To get the “right” shapes, we show that all the families that are born either too early or too late, or have a fitness that is too small have a renormalised size that goes to zero. More precisely:

▶ **Lemma 16.** *Let $\eta, \varepsilon > 0$. There exists $\kappa_1 = \kappa_1(\varepsilon, \eta)$ such that*

$$\liminf_{t\to\infty} \mathbb{P}\Big(\Gamma_t\big([-\infty,\infty]\times[-\infty,-\kappa_1]\times(\varepsilon,\infty]\big)=0\Big) \geq 1-\eta.$$

There exists $v = v(\varepsilon, \eta) > 1$ such that

$$\liminf_{t\to\infty} \mathbb{P}\Big(\Gamma_t\big([-\infty,-v]\cup[v,\infty]\times[-\infty,\infty]\times(\varepsilon,\infty]\big)=0\Big) \geq 1-\eta.$$

And, finally, there exists $\kappa_2 = \kappa_2(\varepsilon, \eta)$ such that

$$\liminf_{t\to\infty} \mathbb{P}\Big(\Gamma_t\big([-v,v]\times[\kappa_2,\infty]\times(\varepsilon,\infty]\big)=0\Big) \geq 1-\eta.$$

This lemma is proved in [5, Sec. 4]. Proposition 15 then gives that Γ_t converges on $(-v,v)\times(-\kappa_1,\kappa_2)\times(\varepsilon,\infty]$ to the Poisson process with intensity measure ζ. Combining this with Lemma 16 and using that $\eta > 0$ is arbitrarily small, we get convergence on $[-\infty,\infty]\times[-\infty,\infty]\times(\varepsilon,\infty]$. The fact that this holds for all $\varepsilon > 0$ concludes the proof.

Sketch of the proof of Proposition 15

The proof of Proposition 15 is done in two steps: First we prove convergence of the following Poisson process, whose only difference with Γ_t is the last coordinate, which has been replaced by a quantity that, by Assumption **(A3)**, converges almost surely to a ν-distributed random variable:

▶ **Proposition 17.** *We have vague convergence in distribution of the point process*

$$\Psi_t = \sum_{n=1}^{M(t)} \delta\Big(\frac{\tau_n-\sigma_t}{\sqrt{\sigma_t}}, \frac{F_n - g\big(\log(n\sqrt{\sigma_t})\big)}{g'\big(\log(n\sqrt{\sigma_t})\big)}, \mathrm{e}^{-\gamma F_n(t-\tau_n)} Z_n(t)\Big)$$

to the Poisson point process on $(-\infty,\infty)\times(-\infty,\infty]\times[0,\infty]$ with intensity

$$\zeta^*(\mathrm{d}s,\, \mathrm{d}f,\, \mathrm{d}z) = \lambda \mathrm{e}^{-f}\nu(z)\mathrm{d}s\,\mathrm{d}f\,\mathrm{d}z.$$

This is enough to imply convergence of Γ_t because Γ_t is the image of Ψ_t by a continuous function: we show (see [5, Sec. 3.3]) that, if $\phi\colon (s,f,z)\to(s,f,\mathrm{e}^{-s^2a_2+fa_3}z)$, then $\Psi_t\circ\phi^{-1}$ is asymptotically equivalent to Γ_t, i.e. for all Lipschitz continuous compactly-supported functions $f\colon(-\infty,\infty)\times(-\infty,\infty)\times[0,\infty]\to\mathbb{R}$,

$$\left|\int f\mathrm{d}\Psi_t\circ\phi^{-1} - \int f\mathrm{d}\Gamma_t\right| \to 0 \quad \text{in probability, as } t\uparrow\infty.$$

This, together with Proposition 17, implies that Γ_t converges to the Poisson point process of intensity $\zeta = \zeta^*\circ\phi$, as claimed in Proposition 15.

Sketch of the proof of Proposition 17. The advantage of Ψ_t over Γ_t is that, because of Assumption **(A3)**, the third coordinate converges almost surely to a ν-distributed random variable. In fact, using also the fact that, by Assumption **(A1)**, τ_n is close to $(\log n)/\lambda$, one can show (see [5, Lemma 9]) that Ψ_t is asymptotically equivalent to

$$\Psi_t^* = \sum_{n\in\mathbb{N}} \delta\left(\frac{(\log n)/\lambda - \sigma_t}{\sqrt{\sigma_t}}, \frac{F_n - g\big(\log(n\sqrt{\sigma_t})\big)}{g'\big(\log(n\sqrt{\sigma_t})\big)}, \xi_n\right),$$

where the ξ_n's are i.i.d. random variables of distribution ν. This implies that to prove Proposition 17 it is enough to prove convergence of Ψ_t^* to the Poisson point process of intensity ζ^*. The advantage of Ψ_t^* over Ψ_t is that the three coordinates are three independent sequences of independent random variables: one can thus apply Kallenberg's theorem (see [8, Proposition 3.22]), which says that it is enough to prove that for every precompact relatively-open box $B \subset (-\infty, \infty) \times (-\infty, \infty] \times [0, \infty]$,

(a) $\mathbb{P}(\Psi_t^*(B) = 0) \to \exp(-\zeta^*(B))$, as $t \uparrow \infty$, and
(b) $\mathbb{E}[\Psi_t^*(B)] \to \zeta^*(B)$, as $t \uparrow \infty$.

Conditions **(a)** and **(b)** are checked in [5, Sec. 3.2]: this concludes the proof of Proposition 17 and thus of Proposition 15. ◀

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Convergence Rates in the Probabilistic Analysis of Algorithms

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Abstract

In this extended abstract a general framework is developed to bound rates of convergence for sequences of random variables as they mainly arise in the analysis of random trees and divide-and-conquer algorithms. The rates of convergence are bounded in the Zolotarev distances. Concrete examples from the analysis of algorithms and data structures are discussed as well as a few examples from other areas. They lead to convergence rates of polynomial and logarithmic order. Our results show how to obtain a significantly better bound for the rate of convergence when the limiting distribution is Gaussian.

2012 ACM Subject Classification Theory of computation → Sorting and searching; Theory of computation → Divide and conquer

Keywords and phrases weak convergence, probabilistic analysis of algorithms, random trees, probability metrics

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.22

1 Introduction and notation

In this extended abstract we consider a general recurrence for (probability) distributions which covers many instances of complexity measures of divide-and-conquer algorithms and parameters of random search trees. We consider a sequence $(Y_n)_{n\geq 0}$ of d-dimensional random vectors satisfying the distributional recursion

$$Y_n \stackrel{d}{=} \sum_{r=1}^{K} A_r(n) Y^{(r)}_{I_r^{(n)}} + b_n, \qquad n \geq n_0, \tag{1}$$

where $(A_1(n),\dots,A_K(n),b_n,I^{(n)}),(Y_n^{(1)})_{n\geq 0},\dots,(Y_n^{(K)})_{n\geq 0}$ are independent, the coefficients $A_1(n),\dots,A_K(n)$ are random $(d\times d)$-matrices, b_n is a d-dimensional random vector, $I^{(n)} = (I_1^{(n)},\dots,I_K^{(n)})$ is a random vector in $\{0,\dots,n\}^K$, $n_0 \geq 1$ and $(Y_n^{(r)})_{n\geq 0} \stackrel{d}{=} (Y_n)_{n\geq 0}$ for $r = 1,\dots,K$. Moreover, $K \geq 1$ is a fixed integer, but extensions to K being random and depending on n are possible.

This is the framework of [14] where some general convergence results are shown for appropriate normalizations of the Y_n. The content of the present extended abstract is to also study the rates of convergence in such limit theorems.

We define the normalized sequence $(X_n)_{n\geq 0}$ by

$$X_n := C_n^{-1/2}(Y_n - M_n), \qquad n \geq 0,$$

where M_n is a d-dimensional vector and C_n a positive definite $(d\times d)$-matrix. Essentially, we choose M_n as the mean and C_n as the covariance matrix of Y_n if they exist or as the leading order terms in expansions of these moments as $n\to\infty$. The normalized quantities satisfy the following modified recursion:

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 22; pp. 22:1–22:13
Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

$$X_n \stackrel{d}{=} \sum_{r=1}^{K} A_r^{(n)} X^{(r)}_{I_r^{(n)}} + b^{(n)}, \qquad n \geq n_0, \tag{2}$$

with

$$A_r^{(n)} := C_n^{-1/2} A_r(n) C^{1/2}_{I_r^{(n)}}, \quad b^{(n)} := C_n^{-1/2}\left(b_n - M_n + \sum_{r=1}^{K} A_r(n) M_{I_r^{(n)}}\right) \tag{3}$$

and independence relations as in (1).

In the context of the contraction method the aim is to establish transfer theorems of the following form: After verifying the assumptions of appropriate convergence of the coefficients $A_r^{(n)} \to A_r^*, b^{(n)} \to b^*$ then convergence in distribution of random vectors (X_n) to a limit X is implied. The limit distribution $\mathcal{L}(X)$ is identified by a fixed-point equation obtained from (2) by considering formally $n \to \infty$:

$$X \stackrel{d}{=} \sum_{r=1}^{K} A_r^* X^{(r)} + b^*.$$

Here $(A_1^*, \dots, A_K^*, b^*), X^{(1)}, \dots, X^{(K)}$ are independent and $X^{(r)} \stackrel{d}{=} X$ for $r = 1, \dots, K$.

The aim of the present extended abstract is to endow such general transfer theorems with bounds on the rates of convergence. As a distance measure between (probability) distributions we use the Zolotarev metric. For various of the applications we discuss, bounds on the rate of convergence have been derived one by one for more popular distance measures such as the Kolmogorov–Smirnov distance. However, the transfer theorems of the present paper in terms of the smoother Zolotarev metrics are easy to apply and cover a broad range of applications at once. A crucial role is played by a factor 3 in the exponent of these orders in cases where the normal distribution is the limiting distribution, see Remark 4.

In the rest of this section we fix some notation. Regarding norms of vectors and (random) matrices we denote for $x \in \mathbb{R}^d$ by $\|x\|$ its Euclidean norm and for a random vector X and some $0 < p < \infty$, we set $\|X\|_p := \mathbb{E}[\|X\|^p]^{(1/p)\wedge 1}$. Furthermore, for a $(d \times d)$-matrix A, $\|A\|_{\mathrm{op}} := \sup_{\|x\|=1} \|Ax\|$ denotes the spectral norm of A and for a random such A we define $\|A\|_p := \mathbb{E}[\|A\|_{\mathrm{op}}^p]^{(1/p)\wedge 1}$ for a random square matrix and $0 < p < \infty$. Note that for a symmetric $(d \times d)$-matrix A, we have $\|A\|_{\mathrm{op}} = \max\{|\lambda| : \lambda \text{ eigenvalue of } A\}$. By Id_d the d-dimensional unit matrix is denoted. For multilinear forms the norm is defined similarly.

Furthermore we define by $\mathcal{P}^d$ the space of probability distributions in $\mathbb{R}^d$ (endowed with the Borel σ-field), by $\mathcal{P}_s^d := \{\mathcal{L}(X) \in \mathcal{P}^d : \|X\|_s < \infty\}$ and for a vector $m \in \mathbb{R}^d$, and a symmetric positive semidefinite $(d \times d)$-matrix C the spaces

$$\begin{aligned} \mathcal{P}_s^d(m) &:= \{\mathcal{L}(X) \in \mathcal{P}_s^d : \mathbb{E}[X] = m\}, \quad s > 1, \\ \mathcal{P}_s^d(m, C) &:= \{\mathcal{L}(X) \in \mathcal{P}_s^d : \mathbb{E}[X] = m, \mathrm{Cov}(X) = C\}, \quad s > 2. \end{aligned} \tag{4}$$

We use the convention $\mathcal{P}_s^d(m) := \mathcal{P}_s^d$ for $s \leq 1$ and $\mathcal{P}_s^d(m, C) := \mathcal{P}_s^d(m)$ for $s \leq 2$.

The Zolotarev metrics ζ_s, [19], are defined for probability distributions $\mathcal{L}(X), \mathcal{L}(Y) \in \mathcal{P}^d$ by

$$\zeta_s(X, Y) := \zeta_s(\mathcal{L}(X), \mathcal{L}(Y)) = \sup_{f \in \mathcal{F}_s} |E(f(X) - f(Y))|,$$

where for $s = m + \alpha, 0 < \alpha \leq 1, m \in \mathbb{N}_0$,

$$\mathcal{F}_s := \{f \in C^m(\mathbb{R}^d, \mathbb{R}) : \|f^{(m)}(x) - f^{(m)}(y)\| \leq \|x - y\|^\alpha\}.$$

Note that these distance measures may be infinite. Finite metrics are given by ζ_s on $\mathcal{P}_s^d$ for $0 \leq s \leq 1$, by ζ_s on $\mathcal{P}_s^d(m)$ for $1 < s \leq 2$, and by ζ_s on $\mathcal{P}_s^d(m, C)$ for $2 < s \leq 3$, cf. (4).

2 Results

We return to the situation outlined in the introduction, where we have normalized $(Y_n)_{n\geq 0}$ in the following way:

$$X_n := C_n^{-1/2}(Y_n - M_n), \qquad n \geq 0, \tag{5}$$

where M_n is a d-dimensional random vector and C_n a positive definite $(d \times d)$-matrix. As recalled in Section 1, for $s > 1$, we may fix the mean and covariance matrix of the scaled quantities to guarantee the finiteness of the ζ_s-metric. Therefore, we choose $M_n = \mathbb{E}[Y_n]$ for $n \geq 0$ and $s > 1$. For $s > 2$, we additionally have to control the covariances of X_n. We assume that there exists an $n_1 \geq 0$ such that $\mathrm{Cov}(Y_n)$ is positive definite for $n \geq n_1$ and choose $C_n = \mathrm{Cov}(Y_n)$ for $n \geq n_1$ and $C_n = \mathrm{Id}_d$ for $n < n_1$. For $s \leq 2$, we just assume that C_n is positive definite and set $n_1 = 0$ in this case.

The normalized quantities satisfy the modified recursion

$$X_n \stackrel{d}{=} \sum_{r=1}^{K} A_r^{(n)} X_{I_r^{(n)}}^{(r)} + b^{(n)}, \qquad n \geq n_0,$$

with $A_r^{(n)}$ and $b^{(n)}$ given in (3). The following theorem discusses a general framework to bound rates of convergence for the sequence $(X_n)_{n\geq 0}$. For the proof, we need some technical conditions which guarantee that the sizes $I_r^{(n)}$ of the subproblems grow with n. More precisely, we will assume that there exists some monotonically decreasing sequence $R(n) > 0$ with $R(n) \to 0$ such that

$$\left\|\mathbf{1}_{\{I_r^{(n)} < \ell\}} A_r^{(n)}\right\|_s = \mathrm{O}(R(n)), \quad n \to \infty, \tag{6}$$

for all $\ell \in \mathbb{N}$ and $r = 1, \ldots, K$ and that

$$\left\|\mathbf{1}_{\{I_r^{(n)} = n\}} A_r^{(n)}\right\|_s \to 0, \quad n \to \infty, \tag{7}$$

for all $r = 1, \ldots, K$.

2.1 A general transfer theorem for rates of convergence

Our first result is a direct extension of the main Theorem 4.1 in [14], where we essentially only make all the estimates there explicit. The main result of the present extended abstract is contained in Section 2.2.

▶ **Theorem 1.** *Let $(X_n)_{n\geq 0}$ be L_s-integrable, $0 < s \leq 3$, and satisfy recurrence (5) with the choices for M_n and C_n specified there. We assume that there exist s-integrable $A_1^*, \ldots, A_K^*, b^*$ and some monotonically decreasing sequence $R(n) > 0$ with $R(n) \to 0$ such that, as $n \to \infty$,*

$$\left\|b^{(n)} - b^*\right\|_s + \sum_{r=1}^{K} \left\|A_r^{(n)} - A_r^*\right\|_s = \mathrm{O}(R(n)). \tag{8}$$

If conditions (6) and (7) are satisfied and if

$$\limsup_{n\to\infty}\ \mathbb{E}\sum_{r=1}^{K}\left(\frac{R(I_r^{(n)})}{R(n)}\left\|A_r^{(n)}\right\|_{\mathrm{op}}^s\right) < 1, \tag{9}$$

then we have, as $n \to \infty$,

$$\zeta_s(X_n, X) = \mathrm{O}(R(n)),$$

where $\mathcal{L}(X)$ is given as the unique fixed point in $\mathcal{P}_s^d(0, \mathrm{Id}_d)$ of the equation

$$X \stackrel{d}{=} \sum_{r=1}^{K} A_r^* X^{(r)} + b^*, \tag{10}$$

with $(A_1^*, \dots, A_K^*, b^*), X^{(1)}, \dots, X^{(K)}$ independent and $X^{(r)} \stackrel{d}{=} X$ for $r = 1, \dots, K$.

▶ Remark 2. In applications, the convergence rate of the coefficients (conditions (6) and (8)) is often faster than the convergence rate of the quantities X_n, see, e.g., Section 4.4. In these cases, it is often possible to perform the induction step in the proof of Theorem 1 although condition (9) does not hold. To be more precise, we may assume

$$\left\|\mathbf{1}_{\{I_r^{(n)} < \ell\}} A_r^{(n)}\right\|_s + \left\|b^{(n)} - b^*\right\|_s + \left\|A_r^{(n)} - A_r^*\right\|_s = \mathrm{O}(\widetilde{R}(n))$$

for every $\ell \geq 0$, $r = 1, \dots, K$ and $n \to \infty$. Then, instead of condition (9), it is sufficient to find some $K > 0$ such that

$$\mathbb{E}\left[\sum_{r=1}^{K} \mathbf{1}_{\{n_1 \leq I_r^{(n)} < n\}} \frac{R(I_r^{(n)})}{R(n)} \|A_r^{(n)}\|_{\mathrm{op}}^s\right] \leq 1 - p_n - \frac{\widetilde{R}(n)}{K R(n)}$$

for all large n with $p_n := \mathbb{E}\left[\sum_{r=1}^{K} \mathbf{1}_{\{I_r^{(n)} = n\}} \|A_r^{(n)}\|_{\mathrm{op}}^s\right]$.

2.2 An improved transfer theorem for normal limit distributions

We now consider the special case where the sequence $(X_n)_{n\geq 0}$ has finite third moments and satisfies recursion (2) with $(A_1^{(n)}, \dots, A_K^{(n)}, b^{(n)}) \xrightarrow{L_3} (A_1^*, \dots, A_K^*, b^*)$ for some coefficients $A_1^*, \dots, A_K^*, b^*$ with finite third moments and

$$b^* = 0, \quad \sum_{r=1}^{K} A_r^* (A_r^*)^T = \mathrm{Id}_d$$

almost surely. Corollary 3.4 in [14] implies that, if $\mathbb{E}[\sum_{r=1}^{K} \|A_r^*\|_{\mathrm{op}}^3] < 1$, equation (10) has a unique solution in the space $\mathcal{P}_3^d(0, \mathrm{Id}_d)$. Furthermore, e.g., using characteristic functions, it is easily checked that this unique solution is the standard normal distribution $\mathcal{N}(0, \mathrm{Id}_d)$.

In this special case of normal limit laws, it is possible to derive a refined version of Theorem 1. Instead of the technical condition (6), we now need the weaker condition

$$\left\|\mathbf{1}_{\{I_r^{(n)} < \ell\}} A_r^{(n)}\right\|_3^3 = \mathrm{O}(R(n)), \quad n \to \infty, \tag{11}$$

for all $\ell \in \mathbb{N}$ and $r = 1, \dots, K$. Moreover, condition (8) concerning the convergence rates of the coefficients can be weakened, which is formulated in the following theorem.

▶ **Theorem 3.** *Let $(X_n)_{n\geq 0}$ be given as in (5) with finite third moments. We assume that for some $R(n) > 0$ monotonically decreasing with $R(n) \to 0$ as $n \to \infty$ we have*

$$\left\|\sum_{r=1}^{K} A_r^{(n)} (A_r^{(n)})^T - \mathrm{Id}_d\right\|_{3/2}^{3/2} + \left\|b^{(n)}\right\|_3^3 = \mathrm{O}(R(n)), \tag{12}$$

and the technical conditions (7) and (11) being satisfied for $s = 3$. If

$$\limsup_{n\to\infty} \mathbb{E} \sum_{r=1}^{K} \left(\frac{R(I_r^{(n)})}{R(n)} \|A_r^{(n)}\|_{\mathrm{op}}^3\right) < 1, \tag{13}$$

then we have, as $n \to \infty$,

$$\zeta_3(X_n, \mathcal{N}(0, \mathrm{Id}_d)) = \mathrm{O}(R(n)).$$

Proof. (Sketch) We define an accompanying sequence $(Z_n^*)_{n\geq 0}$ by

$$Z_n^* := \sum_{r=1}^{K} A_r^{(n)} T_{I_r^{(n)}} N^{(r)} + b^{(n)}, \qquad n \geq 0,$$

where $(A_1^{(n)}, \dots, A_K^{(n)}, I^{(n)}, b^{(n)}), N^{(1)}, \dots, N^{(K)}$ are independent, $\mathcal{L}(N^{(r)}) = \mathcal{N}(0, \mathrm{Id}_d)$ for $r = 1, \dots, K$ and $T_n T_n^T = \mathrm{Cov}(X_n)$ for $n \geq 0$. Hence, Z_n^* has a finite third moment, $\mathbb{E}[Z_n^*] = 0$ and $\mathrm{Cov}(Z_n^*) = \mathrm{Id}_d$ for all $n \geq n_1$. By the triangle inequality, we have

$$\zeta_3(X_n, \mathcal{N}(0, \mathrm{Id}_d)) \leq \zeta_3(X_n, Z_n^*) + \zeta_3(Z_n^*, \mathcal{N}(0, \mathrm{Id}_d)).$$

Then, the assertion follows inductively if one has shown the bound $\zeta_3(Z_n^*, \mathcal{N}(0, \mathrm{Id}_d)) = \mathrm{O}(R(n))$: Using the convolution property of the multidimensional normal distribution, we obtain the representation

$$Z_n^* = \sum_{r=1}^{K} A_r^{(n)} T_{I_r^{(n)}} N^{(r)} + b^{(n)} \stackrel{d}{=} G_n N + b^{(n)},$$

where $G_n G_n^T = \sum_{r=1}^K A_r^{(n)} T_{I_r^{(n)}} T_{I_r^{(n)}}^T (A_r^{(n)})^T$, $\mathcal{L}(N) = \mathcal{N}(0, \mathrm{Id}_d)$ and N is independent of $(G_n, b^{(n)})$. As $\mathrm{Cov}(Z_n^*) = \mathrm{Id}_d$ for all $n \geq n_1$, we have $\mathbb{E}[G_n G_n^T + b^{(n)} (b^{(n)})^T] = \mathrm{Id}_d$ for $n \geq n_1$. Furthermore, we have $\|b^{(n)}\|_3^3 = \mathrm{O}(R(n))$ and

$$\begin{aligned}
\left\|G_n G_n^T - \mathrm{Id}_d\right\|_{3/2}^{3/2} &= \left\| \sum_{r=1}^{K} A_r^{(n)} T_{I_r^{(n)}} T_{I_r^{(n)}}^T (A_r^{(n)})^T - \mathrm{Id}_d \right\|_{3/2}^{3/2} \\
&= \mathrm{O}\Bigg(\left\| \sum_{r=1}^{K} \mathbf{1}_{\{I_r^{(n)} < n_1\}} A_r^{(n)} (T_{I_r^{(n)}} T_{I_r^{(n)}}^T - \mathrm{Id}_d)(A_r^{(n)})^T \right\|_{3/2}^{3/2} \\
&\qquad + \left\| \sum_{r=1}^{K} A_r^{(n)} (A_r^{(n)})^T - \mathrm{Id}_d \right\|_{3/2}^{3/2} \Bigg) \\
&= \mathrm{O}\left(\sum_{r=1}^{K} \left\| \mathbf{1}_{\{I_r^{(n)} < n_1\}} A_r^{(n)} \right\|_3^3 + \left\| \sum_{r=1}^{K} A_r^{(n)} (A_r^{(n)})^T - \mathrm{Id}_d \right\|_{3/2}^{3/2} \right) \\
&= \mathrm{O}(R(n)).
\end{aligned}$$

Thus, the following Lemma 5 implies $\zeta_3(Z_n^*, \mathcal{N}(0, \mathrm{Id}_d)) = \mathrm{O}(R(n))$. Lemma 5 is the main part of the present proof. ◀

▶ Remark 4. Theorem 3, when applicable, often improves over Theorem 1 by a factor 3 in the exponent, see Remark 9 for an example. This is caused by the additional exponents in (12) in comparison to (8).

▶ **Lemma 5.** *Let $(Z_n^*)_{n\geq 0}$ be a sequence of d-dimensional random vectors satisfying $Z_n^* \stackrel{d}{=} G_n N + b^{(n)}$ with some random $(d \times d)$-matrix G_n and some random vector $b^{(n)}$ such that $\mathbb{E}[Z_n^*] = 0$, $\mathrm{Cov}(Z_n^*) = \mathrm{Id}_d$ and $N \sim \mathcal{N}(0, \mathrm{Id}_d)$ is independent of $(G_n, b^{(n)})$. Furthermore, we assume that, as $n \to \infty$,*

$$\left\|G_n G_n^T - \mathrm{Id}_d\right\|_{3/2}^{3/2} + \left\|b^{(n)}\right\|_3^3 = \mathrm{O}(R(n))$$

for appropriate $R(n)$. Then, we have, as $n \to \infty$,

$$\zeta_3(Z_n^*, \mathcal{N}(0, \mathrm{Id}_d)) = \mathrm{O}(R(n)).$$

The proof of Lemma 5 builds upon ideas of [15].

3 Expansions of moments

In applications to problems arising in theoretical computer science, where the recurrence (1) is explicitly given, one usually has no direct means to identify the orders of the terms $\|b^{(n)} - b^*\|_s$ and $\|A_r^{(n)} - A_r^*\|_s$. This is due to the fact that the mean vector M_n and the covariance matrix C_n, for the cases $1 < s \le 2$ and $2 < s \le 3$ respectively, which are used for the normalization (5) are typically not exactly known or too involved to be amenable to explicit calculations. As a substitute one usually has asymptotic expansions of these sequences as $n \to \infty$.

In the present section we assume the dimension to be $d = 1$ and $A_r(n) = 1$ for all $r = 1, \dots, K$ and provide tools to apply the general Theorems 1 and 3 on the basis of expansions of the mean and variance. We assume that

$$\mathbb{E}[X_n] = \mu(n) = f(n) + \mathrm{O}(e(n)), \quad \mathrm{Var}(X_n) = \sigma^2(n) = g(n) + \mathrm{O}(h(n)), \tag{14}$$

with $e(n) = o(f(n))$ and $h(n) = o(g(n))$. To connect Theorems 1 and 3 to recurrences with known expansions we use the following notion.

▶ **Definition 6.** *A sequence $(a(n))_{n\ge 0}$ of non-negative numbers is called* essentially non-decreasing *if there exists a $c > 0$ such that $a(m) \le ca(n)$ for all $0 \le m < n$.*

The scaling introduced in (5) with the special choices $A_r(n) = 1$ for all $r = 1, \dots, K$ leads to the scaled recurrence for (X_n) given in (2) with

$$A_r^{(n)} = \frac{\sigma(I_r^{(n)})}{\sigma(n)}, \quad b^{(n)} = \frac{1}{\sigma(n)}\Big(b_n - \mu(n) + \sum_{r=1}^K \mu(I_r^{(n)})\Big). \tag{15}$$

Additionally, we consider the corresponding quantities

$$\overline{A}_r^{(n)} = \frac{g^{1/2}(I_r^{(n)})}{g^{1/2}(n)}, \quad \overline{b}^{(n)} = \frac{1}{g^{1/2}(n)}\Big(b_n - f(n) + \sum_{r=1}^K f(I_r^{(n)})\Big). \tag{16}$$

Then we have:

▶ **Lemma 7.** *With $A_r^{(n)}$, $b^{(n)}$ given in (15), $\overline{A}_r^{(n)}$, $\overline{b}^{(n)}$ given in (16), and the expansions for $\mu(n)$, $\sigma^2(n)$ given in (14) the following holds.*
If the sequence $h/g^{1/2}$ is essentially non-decreasing then

$$\big\|A_r^{(n)} - A_r^*\big\|_s \le \big\|\overline{A}_r^{(n)} - A_r^*\big\|_s + \mathrm{O}\Big(\frac{h(n)}{g(n)}\Big). \tag{17}$$

If the sequence h is essentially non-decreasing then

$$\Big\|\sum_{r=1}^K (A_r^{(n)})^2 - 1\Big\|_s \le \Big\|\sum_{r=1}^K (\overline{A}_r^{(n)})^2 - 1\Big\|_s + \mathrm{O}\Big(\frac{h(n)}{g(n)}\Big). \tag{18}$$

If the sequence e is essentially non-decreasing then

$$\big\|b^{(n)} - b^*\big\|_s \le \big\|\overline{b}^{(n)} - b^*\big\|_s + \mathrm{O}\Big(\frac{h(n)}{g(n)} + \frac{e(n)}{g^{1/2}(n)}\Big). \tag{19}$$

If the sequence g/h is essentially non-decreasing and

$$T(n) := \mathbb{E}\sum_{r=1}^K \frac{g^{s/2-1}(I_r^{(n)})h(I_r^{(n)})R(I_r^{(n)})}{g^{s/2}(n)R(n)}$$

then we have

$$\mathbb{E}\sum_{r=1}^K \frac{\sigma^s(I_r^{(n)})R(I_r^{(n)})}{\sigma^s(n)R(n)} \le \mathbb{E}\sum_{r=1}^K \frac{g^{s/2}(I_r^{(n)})R(I_r^{(n)})}{g^{s/2}(n)R(n)} + \mathrm{O}(T(n)). \tag{20}$$

Proof. We show (17), the other bounds can be shown similarly. Note that $\sigma^2(n) = g(n) + \mathrm{O}(h(n))$ implies $\sigma(n) = g^{1/2}(n) + \mathrm{O}(h(n)/g^{1/2}(n))$ and that for any essentially non-decreasing sequence $(a(n))_{n\geq 0}$ we have $\|a(I_r^{(n)})\|_\infty = \mathrm{O}(a(n))$. Since $h/g^{1/2}$ is essentially non-decreasing we obtain

$$\begin{aligned}
A_r^{(n)} = \frac{\sigma(I_r^{(n)})}{\sigma(n)} &= \frac{g^{1/2}(I_r^{(n)}) + \mathrm{O}(h(I_r^{(n)})/g^{1/2}(I_r^{(n)}))}{\sigma(n)} \\
&= \frac{g^{1/2}(I_r^{(n)}) + \mathrm{O}(h(n)/g^{1/2}(n))}{g^{1/2}(n)} \cdot \frac{g^{1/2}(n)}{\sigma(n)} \\
&= \left(\frac{g^{1/2}(I_r^{(n)})}{g^{1/2}(n)} + \mathrm{O}\left(\frac{h(n)}{g(n)}\right)\right)\left(1 + \mathrm{O}\left(\frac{h(n)}{g(n)}\right)\right) \\
&= \frac{g^{1/2}(I_r^{(n)})}{g^{1/2}(n)} + \mathrm{O}\left(\frac{h(n)}{g(n)}\left(1 + \frac{g^{1/2}(I_r^{(n)})}{g^{1/2}(n)}\right)\right).
\end{aligned}$$

Hence, we obtain

$$\|A_r^{(n)} - A_r^*\|_s \leq \|\overline{A}_r^{(n)} - A_r^*\|_s + \mathrm{O}\left(\frac{h(n)}{g(n)}\left(1 + \left\|\overline{A}_r^{(n)}\right\|_s\right)\right).$$

Since $\overline{A}_r^{(n)} \to A_r^*$ in L_s we have $\|\overline{A}_r^{(n)}\|_s = \mathrm{O}(1)$, hence

$$\|A_r^{(n)} - A_r^*\|_s \leq \|\overline{A}_r^{(n)} - A_r^*\|_s + \mathrm{O}\left(\frac{h(n)}{g(n)}\right),$$

which is bound (17). ◀

Note that in applications the terms on the right hand side in the estimates (17)–(20) can easily be bounded when expansions as in (14) with explicit functions e, f, g, h are available.

4 Applications

We start by deriving a known result to illustrate in detail how to apply our framework of the previous sections.

4.1 Quicksort: Key comparisons

The number of key comparisons Y_n needed by the Quicksort algorithm to sort n randomly permuted (distinct) numbers satisfies the distributional recursion

$$Y_n \stackrel{d}{=} Y_{I_n} + Y'_{n-1-I_n} + n - 1, \quad n \geq 1, \tag{21}$$

where $Y_0 := 0$ and $(Y_k)_{k=0,\dots,n-1}, (Y'_k)_{k=0,\dots,n-1}, I_n$ are independent, I_n is uniformly distributed on $\{0,\dots,n-1\}$, and $Y_k \stackrel{d}{=} Y'_k$, $k \geq 0$. Hence, equation (21) is covered by our general recurrence (1). For the expectation and variance of Y_n exact expressions are known which imply the asymptotic expansions

$$\begin{aligned}
\mathbb{E}Y_n &= 2n\log(n) + (2\gamma - 4)n + \mathrm{O}(\log n), \\
\mathrm{Var}(Y_n) &= \sigma^2 n^2 - 2n\log(n) + \mathrm{O}(n),
\end{aligned}$$

where γ denotes Euler's constant and $\sigma := \sqrt{7 - 2\pi^2/3} > 0$. We introduce the normalized quantities $X_0 := X_1 := X_2 := 0$ and

$$X_n := \frac{Y_n - \mathbb{E}Y_n}{\sqrt{\mathrm{Var}(Y_n)}}, \quad n \geq 3.$$

To apply Theorem 1 we need to find an $0 < s \le 3$ and a sequence $(R(n))$ with (8) and (9). Note that the Y_n are bounded, thus L_s-integrable for any $s > 0$. To bound the L_s-norms appearing in (8) we use Lemma 7 and choose

$$f(n) = 2n\log(n) + (2\gamma - 4)n, \quad e(n) = \log n,$$
$$g(n) = \sigma^2 n^2, \quad h(n) = n\log n.$$

With these functions we obtain for the quantities defined in (16) that

$$\overline{A}_1^{(n)} = \frac{I_n}{n}, \quad \overline{A}_2^{(n)} = \frac{n-1-I_n}{n},$$
$$\overline{b}^{(n)} = \frac{1}{\sigma}\left(2\frac{I_n}{n}\log\frac{I_n}{n} + 2\frac{n-1-I_n}{n}\log\frac{n-1-I_n}{n} + \frac{n-1}{n} + \mathrm{O}\left(\frac{\log n}{n}\right)\right).$$

With the embedding $I_n = \lfloor nU \rfloor$ with U uniformly distributed over the unit interval $[0,1]$ we have

$$A_1^* = U, \quad A_2^* = 1-U, \quad b^* = \frac{1}{\sigma}\left(2U\log(U) + 2(1-U)\log(1-U) + 1\right) =: \frac{1}{\sigma}\varphi(U).$$

The limit theorem $X_n \to X$ has been derived by different methods by Régnier [16] and Rösler [17]. Rösler [17] also found that the scaled limit $Y := \sigma X$ satisfies the distributional fixed-point equation

$$Y \stackrel{d}{=} UY + (1-U)Y' + \varphi(U).$$

Lower and upper bounds for the rate of convergence in $X_n \to X$ have been studied for various metrics in Fill and Janson [6] and Neininger and Rüschendorf [13].

Now, we apply the framework of the present paper: For $r = 1, 2$ and any $s \ge 1$ we find that

$$\|\overline{A}_r^{(n)} - A_r^*\|_s = \mathrm{O}\Big(\frac{1}{n}\Big).$$

Using Proposition 3.2 of Rösler [17] we obtain

$$\|\overline{b}^{(n)} - b^*\|_s = \mathrm{O}\Big(\frac{\log n}{n}\Big).$$

Moreover, we have

$$\frac{h(n)}{g(n)} = \mathrm{O}(R(n)) \quad \text{and} \quad \frac{e(n)}{g^{1/2}(n)} = \mathrm{O}(R(n)) \quad \text{with} \quad R(n) := \frac{\log n}{n},$$

thus Lemma 7 implies that condition (8) is satisfied for our choice of the sequence R. To verify condition (9) by use of (20) we obtain that for $T(n)$ given in Lemma 7 we find $T(n) = \mathrm{O}(\log(n)/n) \to 0$ and that

$$\mathbb{E}\sum_{r=1}^{2}\frac{g^{s/2}(I_r^{(n)})R(I_r^{(n)})}{g^{s/2}(n)R(n)} = \mathbb{E}\sum_{r=1}^{2}\left(\frac{I_r^{(n)}}{n}\right)^{s-1}\frac{\log I_r^{(n)}}{\log n}.$$

Note that the latter expression has a limit superior of less than 1 if and only if $s > 2$. Hence, Theorem 1 is applicable for $s > 2$ and yields that

$$\zeta_s(X_n, X) = \mathrm{O}\left(\frac{\log n}{n}\right), \quad \text{for} \quad 2 < s \le 3. \tag{22}$$

The bound (22) had previously been shown for $s = 3$ in [13], where also the optimality of the order was shown, i.e., that $\zeta_3(X_n, X) = \Theta(\log(n)/n)$.

In the planned full paper version we also discuss bounds on rates of convergence for various cost measures of the related Quickselect algorithms under various models for the rank to be selected.

4.2 Size of m-ary search trees

The size of m-ary search trees satisfies the recurrence (1) with $K = m \geq 3$, $A_1(n) = \cdots = A_m(n) = 1$, $n_0 = m$, $b_n = 1$, i.e., we have

$$Y_n \stackrel{d}{=} \sum_{r=1}^{m} Y^{(r)}_{I_r^{(n)}} + 1, \quad n \geq m.$$

For a representation of $I^{(n)}$ we define for independent, identically unif$[0,1]$ distributed random variables $U_1, \dots, U_{m-1}$ their spacings in $[0,1]$ by $S_1 = U_{(1)}, S_2 = U_{(2)} - U_{(1)}, \dots, S_m := 1 - U_{(m-1)}$, where $U_{(1)}, \dots, U_{(m-1)}$ denote the order statistics of $U_1, \dots, U_{m-1}$. Then $I^{(n)}$ has the mixed multinomial distribution:

$$I^{(n)} \stackrel{d}{=} M(n - m + 1, S_1, \dots, S_m).$$

By this we mean that given $(S_1, \dots, S_m) = (s_1, \dots, s_m)$ we have that $I^{(n)}$ is multinomial $M(n - m + 1, s_1, \dots, s_m)$ distributed. Expectations, variances and limit laws for Y_n have been studied, see [12, 4]. We have

$$\mathbb{E}Y_n = \mu n + \mathrm{O}(1 + n^{\alpha-1}), \quad m \geq 3, \tag{23}$$

$$\mathrm{Var}(Y_n) = \sigma^2 n + \mathrm{O}(1 + n^{2\alpha-2}), \quad 3 \leq m \leq 26, \tag{24}$$

Here, the constants $\mu, \sigma > 0$ depend on m and $\alpha \in \mathbb{R}$ depends on m such that $\alpha < 1$ for $m \leq 13$, $1 \leq \alpha \leq 4/3$ for $14 \leq m \leq 19$, and $4/3 \leq \alpha \leq 3/2$ for $20 \leq m \leq 26$, see, e.g., Mahmoud [12, Table 3.1] for the values $\alpha = \alpha_m$ depending on m. It is known that Y_n standardized by mean and variance satisfies a central limit law for $m \leq 26$, whereas the standardized sequence has no weak limit for $m > 26$ due to dominant periodicities, see Chern and Hwang [4]. The rate of convergence in the central limit law for $m \leq 26$ for the Kolmogorov metric has been identified in Hwang [9]. Our Theorem 3 implies the central limit theorem for Y_n with $m \leq 26$ with the same (up to an ε for $3 \leq m \leq 19$) rate of convergence for the Zolotarev metric ζ_3:

▶ **Theorem 8.** *The size Y_n of a random m-ary search tree with n items inserted satisfies, for $m \leq 26$ and any $\varepsilon > 0$,*

$$\zeta_3\Big(\frac{Y_n - \mathbb{E}Y_n}{\sqrt{\mathrm{Var}(Y_n)}}, \mathcal{N}(0,1)\Big) = \begin{cases} \mathrm{O}\big(n^{-1/2+\varepsilon}\big), & 3 \leq m \leq 19, \\ \mathrm{O}\big(n^{-3(3/2-\alpha)}\big), & 20 \leq m \leq 26, \end{cases}$$

as $n \to \infty$.

Proof. In order to apply Theorem 3 we have to estimate the orders of $\| \sum_{r=1}^m (A_r^{(n)})^2 - 1\|_{3/2}$ and $\|b^{(n)}\|_3$ with $A_r^{(n)}$ and $b^{(n)}$ defined in (3). For this we apply Lemma 7. From (23) and (24) we obtain that for the quantities appearing in Lemma 7 we can choose $f(n) = \mu n$, $e(n) = 1 \vee n^{\alpha-1}$, $g(n) = \sigma^2 n$, and $h(n) = 1 \vee n^{2(\alpha-1)}$. Hence we obtain

$$\Big\| \sum_{r=1}^{m} (\overline{A}_r^{(n)})^2 - 1 \Big\|_{3/2} = \Big\| \sum_{r=1}^{m} \frac{I_r^{(n)}}{n} - 1 \Big\|_{3/2} = \frac{m-1}{n} = \mathrm{O}\big(n^{-1}\big)$$

and $\mathrm{O}(h(n)/g(n)) = \mathrm{O}(n^{-(1 \wedge (3-2\alpha))})$. This implies

$$\Big\| \sum_{r=1}^{m} (A_r^{(n)})^2 - 1 \Big\|_{3/2}^{3/2} = \mathrm{O}\big(n^{-((3/2) \wedge (3(3/2-\alpha)))}\big).$$

Similarly we obtain

$$\|\bar{b}^{(n)}\|_3 = \frac{1}{\sigma\sqrt{n}}\Big\|1 - \mu n + \sum_{r=1}^{m} \mu I_r^{(n)}\Big\|_3 = \frac{1}{\sigma\sqrt{n}}\big\|1 - \mu(m-1)\big\|_3 = \mathrm{O}\big(n^{-1/2}\big)$$

and $\mathrm{O}(e(n)/g^{1/2}(n)) = \mathrm{O}(n^{-(1/2\wedge(3/2-\alpha))})$. This implies

$$\|b^{(n)}\|_3^3 = \mathrm{O}\big(n^{-((3/2)\wedge(3(3/2-\alpha)))}\big).$$

Hence, condition (12) is satisfied with $R(n) = n^{-((3/2)\wedge(3(3/2-\alpha)))}$. ◀

▶ Remark 9. Using Theorem 1 instead of Theorem 3 in the latter proof is also possible but leads to a bound $\mathrm{O}(n^{-(3/2-\alpha)})$ for $20 \leq m \leq 26$, missing the factor 3 appearing in Theorem 8.

In the full paper version we also discuss rates of convergence for the number of leaves of d-dimensional random point quadtrees in the model of [7, 3, 8] where a similar behavior as in Theorem 8 appears. A technically related example is the number of maxima in right triangles in the model of [1, 2], where the order $n^{-1/4}$ appears. Our framework also applies.

4.3 Periodic functions in mean and variance

We now discuss some applications where the asymptotic expansions of the mean and the variance include periodic functions instead of fixed constants. This is the case for several quantities in binomial splitting processes such as tries, PATRICIA tries and digital search trees. Throughout this section, we assume that we have a sequence $(Y_n)_{n\geq 0}$ with finite third moments satisfying the recursion

$$Y_n \stackrel{d}{=} Y^{(1)}_{I_1^{(n)}} + Y^{(2)}_{I_2^{(n)}} + b_n, \quad n \geq n_0, \tag{25}$$

with $(I^{(n)}, b_n), (Y_n^{(1)})_{n\geq 0}$ and $(Y_n^{(2)})_{n\geq 0}$ independent and $(Y_n^{(r)})_{n\geq 0} \stackrel{d}{=} (Y_n)_{n\geq 0}$ for $r = 1, 2$. Furthermore, $I_1^{(n)}$ has the binomial distribution $\mathrm{Bin}(n, \frac{1}{2})$ and $I_2^{(n)} = n - I_1^{(n)}$ or $I_1^{(n)}$ is binomially $\mathrm{Bin}(n-1, \frac{1}{2})$ distributed and $I_2^{(n)} = n-1-I_1^{(n)}$. Mostly, these binomial recurrences are asymptotically normally distributed, see [10, 11, 14, 18] for some examples.

Our first theorem covers the case of linear mean and variance, i.e. we assume that, as $n \to \infty$,

$$\mathbb{E}[Y_n] = nP_1(\log_2 n) + \mathrm{O}(1), \tag{26}$$

$$\mathrm{Var}(Y_n) = nP_2(\log_2 n) + \mathrm{O}(1), \tag{27}$$

for some smooth and 1-periodic functions P_1, P_2 with $P_2 > 0$. Possible applications would start with the analysis of the number of internal nodes of a trie for n strings in the symmetric Bernoulli model and the number of leaves in a random digital search tree, see, e.g., [10].

▶ **Theorem 10.** *Let $(Y_n)_{n\geq 0}$ have finite third moments and satisfy (25) with $\|b_n\|_3 = \mathrm{O}(1)$, (26) and (27). Then, for any $\varepsilon > 0$ and $n \to \infty$, we have*

$$\zeta_3\Big(\frac{Y_n - \mathbb{E}[Y_n]}{\sqrt{\mathrm{Var}(Y_n)}}, \mathcal{N}(0,1)\Big) = \mathrm{O}(n^{-1/2+\varepsilon}).$$

We now consider the case where our quantities Y_n satisfy recursion (25) with b_n being essentially n. We assume that, as $n \to \infty$, we have

$$\mathbb{E}[Y_n] = n\log_2(n) + nP_1(\log_2 n) + \mathrm{O}(1), \tag{28}$$
$$\mathrm{Var}(Y_n) = nP_2(\log_2 n) + \mathrm{O}(1), \tag{29}$$

for some smooth and 1-periodic functions P_1, P_2 with $P_2 > 0$. This covers, for example, the external path length of random tries and related digital tree structures constructed from n random binary strings under appropriate independence assumptions.

▶ **Theorem 11.** *Let $(Y_n)_{n\ge 0}$ have finite third moments and satisfy (25) with $\|b_n - n\|_3 = \mathrm{O}(1)$, (28) and (29). Then, for any $\varepsilon > 0$ and $n \to \infty$, we have*

$$\zeta_3\Big(\frac{Y_n - \mathbb{E}[Y_n]}{\sqrt{\mathrm{Var}(Y_n)}}, \mathcal{N}(0,1)\Big) = \mathrm{O}(n^{-1/2+\varepsilon}).$$

4.4 A multivariate application

We consider a random binary search tree with n nodes built from a random permutation of $\{1,\dots,n\}$. For $n \ge 0$, we denote by L_{0n} the number of nodes with no left descendant and by L_{1n} the number of nodes with exactly one left descendant. Defining $Y_n := (L_{0n}, L_{1n})$, we have $Y_0 = (0,0)$ and we obtain the following distributional recurrence:

$$Y_n \stackrel{d}{=} Y^{(1)}_{I_1^{(n)}} + Y^{(2)}_{I_2^{(n)}} + b_n, \qquad n \ge 1,$$

where $(Y_j^{(1)})_{j\ge 0}$ and $(Y_j^{(2)})_{j\ge 0}$ are independent copies of $(Y_j)_{j\ge 0}$, $I_1^{(n)}$ is uniformly distributed on $\{0,\dots,n-1\}$ and independent of $(Y^{(1)})$ and $(Y^{(2)})$, $I_2^{(n)} = n-1-I_1^{(n)}$ and $b_n = (\mathbf{1}_{\{I_1^{(n)}=0\}}, \mathbf{1}_{\{I_1^{(n)}=1\}})$. In Devroye [5] it is shown that, for $n \ge 2$,

$$\mathbb{E}[L_{0n}] = \frac{1}{2}(n+1), \quad \mathbb{E}[L_{1n}] = \frac{1}{6}(n+1),$$

and that the standardized quantities have a limiting normal distribution. Using Devroye's description with local counters one also obtains the covariance structure:

▶ **Lemma 12.** *For $n \ge 4$, we have $\mathrm{Cov}(Y_n) = (n+1)\,\Gamma$ with*

$$\Gamma = \frac{1}{360}\begin{pmatrix} 30 & -15 \\ -15 & 28 \end{pmatrix}.$$

For $n \ge 0$, we now set $M_n := \mathbb{E}[Y_n]$, $C_n = \mathrm{Id}_2$ for $n \le 3$, $C_n := \mathrm{Cov}(Y_n)$ for $n \ge 4$ and define $X_n := C_n^{-1/2}(Y_n - M_n)$ for $n \ge 0$. Note that the matrix Γ in Lemma 12 is symmetric and positive definite, which implies, for $n \ge 4$,

$$C_n^{1/2} = \sqrt{n+1}\,\Gamma^{1/2} \quad \text{and} \quad C_n^{-1/2} = \frac{1}{\sqrt{n+1}}\,\Gamma^{-1/2}.$$

The normalized quantities satisfy $X_0 = (0,0)$ and recursion (2) with $K = 2$, $n_0 = 1$,

$$A_r^{(n)} = C_n^{-1/2} C^{1/2}_{I_r^{(n)}} = \mathbf{1}_{\{I_r^{(n)} \ge 4\}} \sqrt{\frac{I_r^{(n)}+1}{n+1}}\,\mathrm{Id}_2 + \mathbf{1}_{\{I_r^{(n)} < 4\}} \frac{1}{\sqrt{n+1}}\,\Gamma^{-1/2}$$

for $r = 1, 2$ and

$$b^{(n)} = C_n^{-1/2}(b_n - M_n + M_{I_1^{(n)}} + M_{I_2^{(n)}}).$$

Modeling all quantities on a joint probability space such that $I_1^{(n)}/n$ converges almost surely to a uniform random variable U in $[0,1]$, we have the L_3-convergences $A_1^{(n)} \to \sqrt{U}\ \mathrm{Id}_2$, $A_2^{(n)} \to \sqrt{1-U}\ \mathrm{Id}_2$ and $b^{(n)} \to 0$ as $n \to \infty$. Thus, we are in the situation of Section 2.2 and obtain the limiting equation

$$X \stackrel{d}{=} \sqrt{U} X^{(1)} + \sqrt{1-U} X^{(2)},$$

with U uniformly distributed on $[0,1]$ and $X^{(1)}$, $X^{(2)}$ and U independent. We now check the conditions of Theorem 3. Since $A_1^{(n)}(A_1^{(n)})^T + A_2^{(n)}(A_2^{(n)})^T = \mathrm{Id}_2$ on the event $\{I_1^{(n)}, I_2^{(n)} \geq 4\}$, we obtain, as $n \to \infty$,

$$\begin{aligned}\Big\| \sum_{r=1}^{2} A_r^{(n)}(A_r^{(n)})^T - \mathrm{Id}_2 \Big\|_{3/2}^{3/2} &= \mathrm{O}\bigg(\Big\| \mathbf{1}_{\{I_1^{(n)}<4\}} \Big(\frac{1}{n+1}\,\Gamma^{-1} + \frac{I_2^{(n)}+1}{n+1}\,\mathrm{Id}_2 - \mathrm{Id}_2 \Big) \Big\|_{3/2}^{3/2} \bigg) \\ &= \mathrm{O}\bigg(\mathbb{E}\Big[\mathbf{1}_{\{I_1^{(n)}<4\}} \Big\| \frac{1}{n+1}\,\Gamma^{-1} - \frac{I_1^{(n)}+1}{n+1}\,\mathrm{Id}_2 \Big\|_{\mathrm{op}}^{3/2} \Big] \bigg) \\ &= \mathrm{O}\big(n^{-5/2}\big).\end{aligned}$$

Similarly, we obtain

$$\big\| b^{(n)} \big\|_3^3 = \mathrm{O}(n^{-5/2}).$$

Since we have $\|\mathbf{1}_{\{I_r^{(n)}<\ell\}} A_r^{(n)}\|_3^3 = \mathrm{O}(n^{-5/2})$ for $\ell \in \mathbb{N}$ and $r = 1, 2$, the technical conditions are satisfied. We now use Theorem 3 with $R(n) = n^{-1/2}$. Note that condition (13) is not satisfied for $R(n) = n^{-1/2}$, but we can use the weakened condition stated in Remark 2 to obtain the following result.

▶ **Theorem 13.** *Denoting by $Y_n := (L_{0n}, L_{1n})$ the vector of the numbers of nodes with no and with exactly one left descendant respectively in a random binary search tree with n nodes we have, for $n \to \infty$, that*

$$\zeta_3\big(\mathrm{Cov}(Y_n)^{-1/2}(Y_n - \mathbb{E}[Y_n]), \mathcal{N}(0, \mathrm{Id}_2)\big) = \mathrm{O}(n^{-1/2}).$$

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Hidden Independence in Unstructured Probabilistic Models

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Abstract

We describe a novel way to represent the probability distribution of a random binary string as a mixture having a maximally weighted component associated with independent (though not necessarily identically distributed) Bernoulli characters. We refer to this as the *latent independent weight* of the probabilistic source producing the string, and derive a combinatorial algorithm to compute it. The decomposition we propose may serve as an alternative to the Boolean paradigm of hypothesis testing, or to assess the fraction of uncorrupted samples originating from a source with independent marginal distributions. In this sense, the latent independent weight quantifies the maximal amount of independence contained within a probabilistic source, which, properly speaking, may not have independent marginal distributions.

2012 ACM Subject Classification Mathematics of computing → Probabilistic representations; Mathematics of computing → Dimensionality reduction; Mathematics of computing → Discrete mathematics

Keywords and phrases Bayesian networks, contamination, latent weights, mixture models, independence, symbolic data

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.23

Funding *Antony Pearson*: NSF Graduate Research Fellowship Program Grant No. 2016198773

Acknowledgements We want to thank three anonymous referees for their careful reading and insightful comments that helped improve the quality of our manuscript.

1 Introduction

Consider the Bayesian network [5] in Figure 1, given in [11, Chapter 2]. As the reader may find familiar, each random variable (node) in the network, given the configurations of its parents, is by definition conditionally independent from its non-descendants. Accordingly, the joint probability mass function of the binary random vector (P, T, S, L, X) factorizes as follows:

$$\begin{aligned}\mathbb{P}(P = p, T = t, S = s, L = l, X = x) = \mathbb{P}(P = p) \cdot \mathbb{P}(T = t) \cdot \mathbb{P}(S = s \mid T = t)\\ \cdot \mathbb{P}(L = l \mid P = p, T = t) \cdot \mathbb{P}(X = x \mid L = l).\end{aligned}$$

In particular, the joint distribution of P, T, S, L and X can be encoded with 10 free parameters. Perhaps unexpectedly, however, one can represent this joint distribution as a mixture with a heavily weighted "independent" component. Specifically:

$$\mathbb{P} = 0.94 \cdot Be(0.02) \otimes Be(0.005) \otimes Be(0.6) \otimes Be(0.01) \otimes Be(0.6) + 0.06 \cdot R, \tag{1}$$

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31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 23; pp. 23:1–23:13
LIPICS Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

where $Be(p)$ denotes a Bernoulli distribution with success probability p, the operator $\otimes$ denotes product measures, and R is a "residual" probability distribution over the sample space $\{0,1\}^5$. This decomposition of $\mathbb{P}$ is possible because for each outcome $(p,t,s,l,x) \in \{0,1\}^5$ a computation shows that:

$$\mathbb{P}(P=p, T=t, S=s, L=l, X=x)$$
$$\geq\ 0.94 \cdot 0.02^p\, 0.98^{1-p} \times 0.005^t\, 0.995^{1-t} \times 0.6^l\, 0.4^{1-l} \times 0.01^x\, 0.99^{1-x} \times 0.6^s\, 0.4^{1-s}.$$

The residual distribution R may be obtained solving for it in equation (1). It turns out in this case that R has low entropy (≈ 3.2 bits, compared to the uniform distribution over $\{0,1\}^5$, which has 5 bits of entropy), and gives probability 0 to twelve of the thirty-two outcomes.

The identity in equation (1) means that, conditioned on a hidden event of 94% probability, the presence of lung infiltrates, the outcome of an X-ray and sputum smear, and the status of a patient having tuberculosis or pneumonia will all be rendered independent. Thus, while in a clinical setting, the dependencies encoded in the Bayesian network may be relevant, on the population level, these covariates often behave independently; in particular, most samples from the Bayesian network can be attributed to a much simpler model (with 5 instead of 10 free parameters).

The decomposition in (1) bears the question: *what's the largest weight a product of independent Bernoulli distributions can have as component of* $\mathbb{P}$*?* Remarkably, the marginal distributions of $\mathbb{P}$ are associated with a weight that is significantly smaller than 94%. Indeed, a computation shows that $P \sim Be(0.05)$, $T \sim Be(0.02)$, $S \sim Be(0.6)$, $L \sim Be(0.05)$, and $X \sim Be(0.6)$, and that P admits the mixture representation:

$$\mathbb{P} = \epsilon \cdot Be(0.05) \otimes Be(0.02) \otimes Be(0.6) \otimes Be(0.05) \otimes Be(0.6) + (1-\epsilon) \cdot R',$$

where $\epsilon \approx 0.104$, and R' is a probability distribution that can be determined from the above identity.

In this article we develop the mathematics of the so-called *(latent) independent weight* of an arbitrary joint probability distribution over a sample space of the form $\{0,1\}^d$, with $d \geq 1$ finite. We argue that the independent weight of a probabilistic source describes the largest average fraction of samples from it that can be attributed to (conditionally) independent Bernoulli random variables, and describe an algorithm to compute this weight, along with some heuristics to approximate it.

The independent weight of a probabilistic source is an intrinsic property of it, which can be used as an objective measure of the approximate correctness of the null hypothesis that "the source has independent marginal distributions," which may be nevertheless false (as the example associated with Figure 1). The concept of independent weight may also be used to distill corrupted data from a source with otherwise independent marginal distributions.

1.1 Related Work

The present work may be regarded as a non-trivial specialization of the recent theory developed in [8]. This previous work introduces the concept of the *latent weight* of a probabilistic source (such as $\mathbb{P}$ in the previous example) with respect to a structured class $\mathcal{Q}$ of probability models over a finite sample space. Specifically, the latent weight of a source P with respect to a class $\mathcal{Q}$ of models is defined as [8]:

$$\lambda_{\mathcal{Q}}(P) := \sup\{\lambda \geq 0 \mid P \geq \lambda \cdot Q \text{ for some } Q \in \mathcal{Q}\}. \tag{2}$$

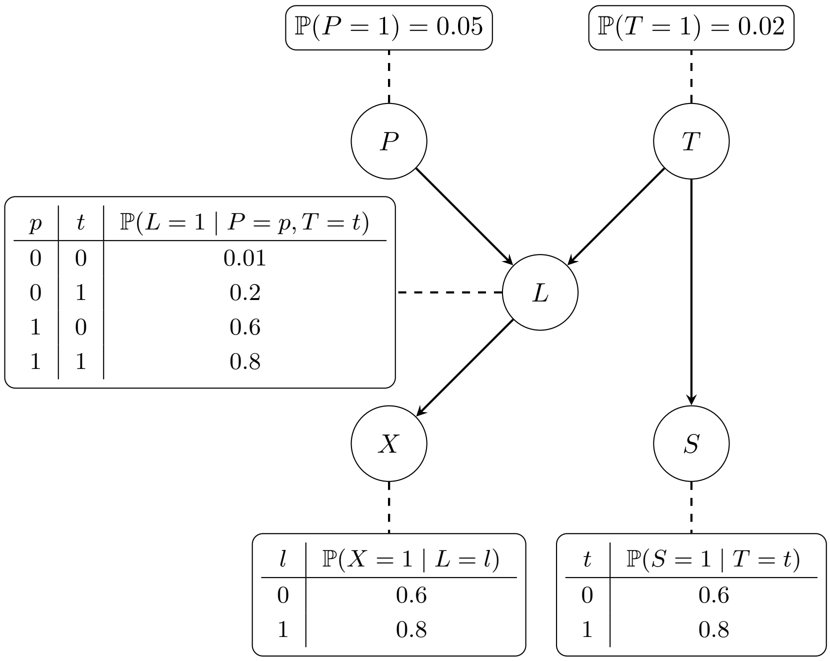

Figure 1 Bayesian network that models the interaction between two lung conditions, tuberculosis (T), and pneumonia (P), and how they jointly affect the probability that a patient will have lung infiltrates (L), the presence of said infiltrates in an X-ray (X), and the outcome of a sputum smear test (S) for tuberculosis. Nodes represent Bernoulli random variables, with conditional probability tables indicated, and the value 1 (0) indicates the presence (absence) of the corresponding condition.

This coefficient represents the largest weight that can be given to a model in $\mathcal{Q}$ as a component in a mixture decomposition of P. In fact, under mild technical conditions, there always exists $Q \in \mathcal{Q}$ and a probabilistic model R such that

$$P = \lambda_{\mathcal{Q}}(P) \cdot Q + (1 - \lambda_{\mathcal{Q}}(P)) \cdot R. \tag{3}$$

Furthermore, when $\mathcal{Q}$ is convex, Q is unique when $\lambda_{\mathcal{Q}}(P) > 0$, and so is R when $\lambda_{\mathcal{Q}}(P) < 1$.

In the current setting, $\mathcal{Q}$ is the class of probability distributions associated with independent binary random variables. We emphasize that much of what we present in this extended abstract may be generalized to more general discrete random variables, however, the binary setting presents enough mathematical challenges to consider it in isolation.

2 Latent Independent Weights

In what follows, $\mathcal{P}$ denotes the set of all probability distributions on $\{0, 1\}^d$, with $d \geq 1$ a given integer. In particular, we may think of elements in $\mathcal{P}$ as non-negative real vectors of dimension 2^d, with entries that sum up to 1.

For $P, Q \in \mathcal{P}$ and $\lambda \in \mathbb{R}$, we write $P \geq \lambda \cdot Q$ to mean that $P(\omega) \geq \lambda \cdot Q(\omega)$, for each $\omega \in \{0, 1\}^d$. Further, we say that Q has *independent marginal distributions* (in short, *independent marginals*) if and only if there are probability distributions $\mu_1, \ldots, \mu_d$ defined over $\{0, 1\}$ such that $Q = \otimes_{i=1}^{d} \mu_i$. Equivalently, Q has independent marginals if and only if it is the probability distribution of a random vector of the form $(X_1, \ldots, X_d)$, with $X_1, \ldots, X_d$ independent (though not necessarily identically distributed) Bernoulli random variables. (In this case, each X_i has distribution μ_i.)

We associate to each $P \in \mathcal{P}$ the real coefficient:

$$\lambda(P) := \lambda_{\mathcal{Q}}(P), \tag{4}$$

where $\lambda_{\mathcal{Q}}(P)$ is as in equation (2) and $\mathcal{Q} \subset \mathcal{P}$ denotes the set of models with independent marginal distributions.

Clearly, $0 \leq \lambda(P) \leq 1$. In fact, according to [8], $\lambda(P) = 1$ if and only if P has independent marginal distributions itself. Furthermore, because the subset of distributions in $\mathcal{P}$ with independent marginal distributions is compact, the supremum in equation (4) is always achieved [8]. Namely, there is $Q \in \mathcal{P}$ with independent marginals such that $P \geq \lambda(P) \cdot Q$. As a result, since $(P - \lambda(P) \cdot Q)$ is a measure with total mass $(1 - \lambda(P))$, there is also $R \in \mathcal{P}$ such that P admits the mixture decomposition:

$$P = \lambda(P) \cdot Q + \big(1 - \lambda(P)\big) \cdot R. \tag{5}$$

This decomposition motivates calling $\lambda(P)$ the *latent independent weight of* P, or simply the *independent weight of* P. It follows that $\lambda(P)$ *is the largest weight that can be attributed to a probability measure over* $\{0,1\}^d$ *with independent marginals as a component of* P. Equivalently: $\lambda(P)$ *is the maximal expected fraction of samples from* P *which may be attributed to a probabilistic source with independent marginal distributions.* More precisely, if $\mathbf{X} = (X_1, \ldots, X_d)$ has distribution P then, up to a hidden event with probability $\lambda(P)$, the Bernoulli random variables $X_1, \ldots, X_d$ are (conditionally) independent.

We note that the model Q with independent marginal distributions in equation (5) is not necessarily unique. For example, let $d = 2$ and P be the uniform distribution over $\{(0,0), (1,1)\}$; in this case, $P = \delta_{(0,0)}/2 + \delta_{(1,1)}/2$, where δ_x is the point probability mass at x. The reader can verify that the only models with independent marginals that can be given positive weight in a probability mixture decomposition of P are $\delta_{(0,0)}$ and $\delta_{(1,1)}$, hence the supremum in equation (4) is achieved by $\delta_{(0,0)}$ as well as $\delta_{(1,1)}$.

2.1 Alternative Formulations

In this section we show how to compute latent independents weights.

Henceforth, $P \in \mathcal{P}$ is assumed fixed. Moreover, we assume that $P > 0$, i.e. $P(\nu) > 0$ for each $\nu \in \{0,1\}^d$. This assumption can be relaxed but goes beyond the scope of this extended abstract.

In what follows, ∞ denotes $+\infty$.

For each $\omega = (\omega_1, \ldots, \omega_d) \in \{0,1\}^d$, let $f_\omega : [0,1]^d \to [1, \infty]$ be the function defined as

$$f_\omega(\mathbf{q}) := \frac{1}{\mathbb{P}(\mathbf{X}_\mathbf{q} = \omega)} = \prod_{i=1}^{d} q_i^{-\omega_i} (1 - q_i)^{\omega_i - 1}, \text{ for } \mathbf{q} = (q_1, \ldots, q_d);$$

where $\mathbf{X}_\mathbf{q} = (X_1, \ldots, X_d)$ is a vector of independent Bernoulli random variables, with $X_i \sim Be(q_i)$. (The second identity above requires to define $0^0 := 1$.) Clearly, $f_\omega(\mathbf{q})$ is a continuous function of $\mathbf{q}$.

For each $\omega \in \{0,1\}^d$, define

$$\mathcal{Q}_\omega := \left\{ \mathbf{q} \in [0,1]^d \,|\, \forall \nu \in \{0,1\}^d : \, P(\omega) f_\omega(\mathbf{q}) \leq P(\nu) f_\nu(\mathbf{q}) \right\}. \tag{6}$$

▶ **Lemma 1.** *If* $P > 0$ *then* $\lambda(P) = \max_{\omega \in \{0,1\}^d} \max_{\mathbf{q} \in \mathcal{Q}_\omega} P(\omega) f_\omega(\mathbf{q})$.

Proof. Since a probability measure over $\{0,1\}^d$ with independent marginal distributions may be represented in terms of d independent Bernoulli random variables, we may restate equation (4) equivalently as follows:

$$\begin{aligned}\lambda(P) &= \sup\left\{\lambda \geq 0 \,\middle|\, \exists \mathbf{q} \in [0,1]^d \, \forall \nu \in \{0,1\}^d : P(\nu) \geq \lambda \cdot \prod_{i=1}^{d} q_i^{\nu_i}(1-q_i)^{1-\nu_i}\right\} \\ &= \sup\left\{\lambda \geq 0 \,\middle|\, \exists \mathbf{q} \in [0,1]^d : \lambda \leq \min_{\nu\in\{0,1\}^d} P(\nu) f_\nu(\mathbf{q})\right\} \\ &= \sup_{\mathbf{q}\in[0,1]^d} \min_{\nu\in\{0,1\}^d} P(\nu) f_\nu(\mathbf{q}) \\ &= \max_{\mathbf{q}\in[0,1]^d} \min_{\nu\in\{0,1\}^d} P(\nu) f_\nu(\mathbf{q}),\end{aligned}$$

where for the second identity we have used that $P > 0$, which prevents the possibility of dealing with anomalous products of the form $0 \cdot \infty$, and for the last identity we have used that $[0,1]^d$ is compact and that the functions f_ν, with $\nu \in \{0,1\}^d$, are continuous.

But observe that for each $\mathbf{q} \in [0,1]^d$ there must exist an ω which minimizes (possibly with ties) the quantity $P(\nu)f_\nu(\mathbf{q})$, with $\nu \in \{0,1\}^d$; that is, $[0,1]^d \subset \cup_{\omega\in\{0,1\}^d} \mathcal{Q}_\omega$. Since, by definition, $\mathcal{Q}_\omega \subset [0,1]^d$ for each ω, we obtain that

$$[0,1]^d = \bigcup_{\omega\in\{0,1\}^d} \mathcal{Q}_\omega.$$

Finally, from the last identity for $\lambda(P)$, the defining property of the set $\mathcal{Q}_\omega$ implies that

$$\lambda(P) = \max_{\omega\in\{0,1\}^d} \max_{\mathbf{q}\in\mathcal{Q}_\omega} \min_{\nu\in\{0,1\}^d} P(\nu) f_\nu(\mathbf{q}) = \max_{\omega\in\{0,1\}^d} \max_{\mathbf{q}\in\mathcal{Q}_\omega} P(\omega) f_\omega(\mathbf{q}). \qquad \blacktriangleleft$$

Lemma 1 reduces the calculation of $\lambda(P)$ to 2^d optimization problems, one for each $\omega \in \{0,1\}^d$, of the form:

$$\max_{\mathbf{q}\in\mathcal{Q}_\omega} P(\omega)\, f_\omega(\mathbf{q}), \text{ with } \omega \in \{0,1\}^d. \tag{7}$$

Our next result aids in making these optimization problems more explicit.

▶ **Lemma 2.** *Assume $P > 0$. For a given $\omega \in \{0,1\}^d$, the transformation $\mathbf{q} \longrightarrow \mathbf{x}$ with $\mathbf{x} = (x_1, \ldots, x_d)$ and $x_i := (\frac{q_i}{1-q_i})^{1-2\omega_i}$, is a bijection between $[0,1]^d$ and $[0,\infty]^d$, and in terms of the variable $\mathbf{x}$:*

$$f_\omega(\mathbf{q}) = \prod_{i=1}^{d}(1+x_i). \tag{8}$$

Under this reparameterization, for each $\mathbf{q} \in (0,1)^d$:

$$\mathbf{q} \in \mathcal{Q}_\omega \textit{ if and only if } \forall \nu \in \{0,1\}^d : \prod_{i:\,\nu_i\neq\omega_i} x_i \leq \frac{P(\nu)}{P(\omega)}, \tag{9}$$

where $\prod_{i:\,\nu_i\neq\omega_i} x_i := 1$ when $\nu = \omega$.

Proof. If $\omega_i = 1$ then $x_i = \frac{1-q_i}{q_i}$, which is a strictly decreasing function of q_i. Instead, if $\omega_i = 0$ then $x_i = \frac{q_i}{1-q_i}$, which is a strictly increasing function of q_i. Thus, in either case, x_i is a strictly monotone function of q_i, with range $[0,\infty]$ when $q_i \in [0,1]$. From this it is immediate that the transformation $\mathbf{q} \to \mathbf{x}$ from $[0,1]^d$ to $[0,\infty]^d$ is one-to-one and onto. On the other hand, if $\omega_i = 1$ then $q_i = \frac{1}{1+x_i}$, hence

$$q_i^{-\omega_i}(1-q_i)^{\omega_i - 1} = \frac{1}{q_i} = 1 + x_i.$$

Likewise, if $\omega_i = 0$ then $q_i = \frac{x_i}{1+x_i}$ i.e. $(1-q_i) = \frac{1}{1+x_i}$, hence

$$q_i^{-\omega_i}(1-q_i)^{\omega_i - 1} = \frac{1}{1-q_i} = 1 + x_i.$$

In either case, $q_i^{-\omega_i}(1-q_i)^{\omega_i-1} = (1+x_i)$, which implies the identity in equation (8).

Because $P > 0$, observe for $\mathbf{q} \in (0,1)^d$ that:

$$\mathbf{q} \in \mathcal{Q}_\omega \text{ if and only if } \forall \nu \in \{0,1\}^d : \frac{f_\omega(\mathbf{q})}{f_\nu(\mathbf{q})} \leq \frac{P(\nu)}{P(\omega)}. \tag{10}$$

But, in terms of the original variable $\mathbf{q}$:

$$\frac{f_\omega(\mathbf{q})}{f_\nu(\mathbf{q})} = \prod_{i=1}^{d} q_i^{\nu_i - \omega_i}(1-q_i)^{\omega_i - \nu_i}.$$

Note however that if $\omega_i = \nu_i$ then $q_i^{\nu_i-\omega_i}(1-q_i)^{\omega_i-\nu_i} = 1$. If instead $\omega_i \neq \nu_i$, there are only two possibilities. On the one hand, if $\omega_i = 0$ and $\nu_i = 1$, then

$$q_i^{\nu_i-\omega_i}(1-q_i)^{\omega_i-\nu_i} = \frac{q_i}{1-q_i} = \left(\frac{q_i}{1-q_i}\right)^{1-2\omega_i} = x_i.$$

On the other hand, if $\omega_i = 1$ and $\nu_i = 0$, then

$$q_i^{\nu_i-\omega_i}(1-q_i)^{\omega_i-\nu_i} = \frac{1-q_i}{q_i} = \left(\frac{q_i}{1-q_i}\right)^{1-2\omega_i} = x_i.$$

As a result:

$$\frac{f_\omega(\mathbf{q})}{f_\nu(\mathbf{q})} = \prod_{i:\nu_i \neq \omega_i} x_i,$$

which together with equation (10) implies the lemma. ◀

The special nature of the constraints in (9), suggests introducing the additional change of variables $\mathbf{x} \to \mathbf{y}$, with $\mathbf{y} = (y_1, \ldots, y_d)$ and $y_i := \ln(x_i)$. The following result is now immediate from the previous lemma.

► **Corollary 3.** *For a given $\omega \in \{0,1\}^d$, the transformation $\mathbf{q} \longrightarrow \mathbf{y}$ with $\mathbf{y} = (y_1, \ldots, y_d)$ and $y_i := (1-2\omega_i) \cdot \ln\left(\frac{q_i}{1-q_i}\right)$, is a bijection between $[0,1]^d$ and $[-\infty,\infty]^d$, and in terms of the variable $\mathbf{y}$:*

$$f_\omega(\mathbf{q}) = \prod_{i=1}^{d}(1+e^{y_i}). \tag{11}$$

Under this reparameterization, for each $\mathbf{q} \in (0,1)^d$:

$$\mathbf{q} \in \mathcal{Q}_\omega \textit{ if and only if } \forall \nu \in \{0,1\}^d : \sum_{i:\,\nu_i \neq \omega_i} y_i \leq \ln\left(\frac{P(\nu)}{P(\omega)}\right), \tag{12}$$

where $\sum_{i:\,\nu_i\neq\omega_i} y_i := 0$ when $\nu = \omega$.

The characterization in equation (12) is not necessarily valid on the boundary of $[0,1]^d$ because, for some $\mathbf{q} \in \partial[0,1]^d$ and different $\omega, \nu \in \{0,1\}^d$, the summation on the right-hand side may be ill-posed due to the simultaneous occurrence of plus and negative infinity terms in the sum. Nevertheless, due to the continuity of f_ω in terms of the variables $\mathbf{q}$ and $\mathbf{y}$ (see equation (11)), if a solution to $\max_{\mathbf{q}\in\mathcal{Q}_\omega} f_\omega(\mathbf{q})$ lives on $\partial[0,1]^d$ then said solution is the limit of points in $\mathcal{Q}_\omega \cap (0,1)^d$. In particular, for each $\omega \in \{0,1\}^d$, the associated optimization problem in equation (7) may be restated in terms of the variable $\mathbf{y}$ as follows:

$$\begin{aligned} &\sup_{\mathbf{y}\in\mathbb{R}^d} && P(\omega)\prod_{i=1}^{d}(1+e^{y_i}) \\ &\text{subject to} && \forall \nu \in \{0,1\}^d : \sum_{i:\,\nu_i\neq\omega_i} y_i \leq \ln\left(\frac{P(\nu)}{P(\omega)}\right). \end{aligned} \tag{13}$$

Each of these new optimization problems has various advantages – compared to the ones in (7). First, up to the factor $P(\omega)$, the objective function does not depend explicitly on ω. Second, the feasible region is a polyhedron [10, Chapter 8], which is a well-studied geometric object. And third, the objective function is monotonically increasing in each coordinate of $\mathbf{y}$; which implies that any solution must lie on the boundary of said polyhedron. We show how to exploit these properties in the next section.

2.2 Geometric Insights

In this section, we fix an outcome $\omega \in \{0,1\}^d$ and describe a combinatorial algorithm to solve the associated optimization problem in equation (13). Define

$$\tilde{\mathcal{Q}}_\omega := \left\{ \mathbf{y}\in\mathbb{R}^d \,\middle|\, \sum_{i:\nu_i\neq\omega_i} y_i \leq \ln\left(\frac{P(\nu)}{P(\omega)}\right) \text{ for each } \nu\in\{0,1\}^d \right\},$$

to denote the feasible region in (13).

In what follows, all vectors are represented as column vectors.

The following result is now immediate from the previous corollary.

▶ **Corollary 4.** *Assume that $P > 0$. For a given $\omega \in \{0,1\}^d$, let A_ω be the binary matrix of dimensions $(2^d-1)\times d$ with entries $A_\omega(\nu,i) := [\![\nu_i \neq \omega_i]\!]$, for each $\nu \in \{0,1\}^d \setminus \{\omega\}$ and $i \in \{1,\ldots,d\}$. Furthermore, let $\mathbf{b}_\omega$ be a column vector of dimension (2^d-1) with entries $\mathbf{b}_\omega(\nu) := \log(P(\nu)/P(\omega))$, for each $\nu \in \{0,1\}^d \setminus \{\omega\}$. Then the feasible region $\tilde{\mathcal{Q}}_\omega$ corresponds to the set of $\mathbf{y} \in \mathbb{R}^d$ satisfying the coordinatewise inequalities:*

$$A_\omega\,\mathbf{y} \leq \mathbf{b}_\omega. \tag{14}$$

The above inequality characterizes $\tilde{\mathcal{Q}}_\omega$ as a non-empty convex polyhedron in $\mathbb{R}^d$. Recall, $\mathbf{y} \in \tilde{\mathcal{Q}}_\omega$ is called a *vertex* if there exists an invertible sub-matrix A'_ω of A_ω of dimensions $d\times d$ and a corresponding sub-vector $\mathbf{b}'_\omega$ of $\mathbf{b}_\omega$ of dimension d such that $A'_\omega\mathbf{y} = \mathbf{b}'_\omega$ [10, Chapter 8, equation (23)]. (The sub-matrix A'_ω and the sub-vector $\mathbf{b}'_\omega$ are associated with the same rows of A_ω and $\mathbf{b}_\omega$, respectively.)

▶ **Lemma 5.** *The polyhedron in equation (14) is pointed, i.e. it contains at least one vertex.*

Proof. For each $i \in \{1, \ldots, d\}$, let $\nu_i \in \{0,1\}^d$ be such that $\nu_i(j) = \omega(j)$ for $j \neq i$, and $\nu_i(i) = 1 - \omega(i)$. Then the sub-matrix of A_ω associated with rows in the set $\{\nu_1, \ldots, \nu_d\}$ corresponds to the $(d \times d)$ identity matrix. As a result, the kernel of A_ω – which coincides exactly with the so-called "lineality space" of the polyhedron – is $\{0\}$, which implies that the polyhedron is pointed [10, Chapter 8, equations (6) and (23)]. ◀

In the language of polyhedral programming, a vertex is a zero-dimensional face. More generally, if $\mathbf{c} \in \mathbb{R}^d \setminus \{0\}$, $\delta \in \mathbb{R}$, and $G := \{\mathbf{y} \in \mathbb{R}^d \mid \mathbf{c}^t\mathbf{y} = \delta\}$ we say the affine hyperplane G is a *supporting hyperplane* of $\tilde{\mathcal{Q}}_\omega$ at the point $\mathbf{y} \in \tilde{\mathcal{Q}}_\omega$ if $\mathbf{y} \in G \cap \tilde{\mathcal{Q}}_\omega$ and $\tilde{\mathcal{Q}}_\omega$ is contained in one of the closed half-spaces bounded by G [7, p. 20]. The non-empty set $F := G \cap \tilde{\mathcal{Q}}_\omega$ is called a *face* of $\tilde{\mathcal{Q}}_\omega$. Equivalently, a face of $\tilde{\mathcal{Q}}_\omega$ is any set of the form $\{\mathbf{y} \in \tilde{\mathcal{Q}}_\omega \mid A'_\omega\mathbf{y} = \mathbf{b}'_\omega\}$, where A'_ω and $\mathbf{b}'_\omega$ are a sub-matrix and sub-vector associated with the same rows of A_ω and $\mathbf{b}_\omega$, respectively [7, Theorem 2.3.3]. (Here, A'_ω does not need to be a square matrix.) The dimension of a face F associated with the subsystem $A'_\omega\mathbf{y} = \mathbf{b}'_\omega$ is $d - \operatorname{rank}(A'_\omega)$.

▶ **Corollary 6.** *If $\mathbf{y} \in \partial\tilde{\mathcal{Q}}_\omega$, the boundary of $\tilde{\mathcal{Q}}_\omega$, and $\mathbf{y}$ is not a vertex of $\tilde{\mathcal{Q}}_\omega$, then $\mathbf{y}$ lies in the relative interior of* some *positive-dimensional face of $\tilde{\mathcal{Q}}_\omega$. That is, there is a positive-dimensional face F and some $\epsilon > 0$ such that the intersection of the closed ϵ-ball around $\mathbf{y}$ and the affine hull of F is contained in F.*

Proof. First, $\tilde{\mathcal{Q}}_\omega$ equals the union of the relative interiors of its faces, which are disjoint [7, Corollary 2.3.7]. In particular:

$$\begin{aligned}\partial\tilde{\mathcal{Q}}_\omega &= \bigsqcup_{\text{faces } F \subsetneqq \tilde{\mathcal{Q}}_\omega} \operatorname{relint}(F) \\ &= \left(\bigsqcup_{\text{non-vertex faces } F \subsetneqq \tilde{\mathcal{Q}}_\omega} \operatorname{relint}(F) \right) \sqcup \left(\bigsqcup_{\text{vertices } v \in \tilde{\mathcal{Q}}_\omega} \{v\} \right),\end{aligned}$$

where $\operatorname{relint}(\cdot)$ denotes the relative interior, and $\sqcup$ denotes a disjoint union. Since a face coincides with its own relative interior if and only if it is a vertex, if $\mathbf{y} \in \partial\tilde{\mathcal{Q}}_\omega$ but $\mathbf{y}$ is not a vertex then $\mathbf{y}$ must lie in the relative interior of a unique positive-dimensional face. ◀

Next we address the optimization problem in equation (13) for a fixed $\omega \in \{0,1\}^d$. Hereafter, we abuse notation slightly and define

$$f_\omega(\mathbf{y}) := \prod_{i=1}^{d} (1 + e^{y_i}),$$

to denote the reparameterized version of $f_\omega(\mathbf{q})$ in terms of the variable $\mathbf{y}$ (see Corollary 3). The following result rules out points in the relative interior of positive-dimensional faces of $\tilde{Q}_\omega$ as maximizers of $f_\omega(\mathbf{y})$.

▶ **Lemma 7.** *Let $F \subset \tilde{\mathcal{Q}}_\omega$ denote a positive-dimensional face of $\tilde{\mathcal{Q}}_\omega$, and $\hat{\mathbf{y}}$ denote a point in the relative interior of F. Then $f_\omega(\hat{\mathbf{y}}) < \max_{\mathbf{y} \in \tilde{\mathcal{Q}}_\omega} f_\omega(\mathbf{y})$. More specifically:*

1. *If the gradient $\nabla f_\omega(\hat{\mathbf{y}})$ is not orthogonal to F, then f_ω can be strictly increased on F, that is, there is some $\hat{\mathbf{z}} \in F$ such that $f_\omega(\hat{\mathbf{z}}) > f_\omega(\hat{\mathbf{y}})$.*
2. *If the gradient $\nabla f_\omega(\hat{\mathbf{y}})$ is orthogonal to F, then $f_\omega(\hat{\mathbf{y}})$ is a local minimum on F.*

Proof. Clearly, f_ω has continuous partial derivatives of any order.

First observe that

$$\frac{\partial f_\omega}{\partial y_i}(\mathbf{y}) = e^{y_i} \prod_{j \neq i} (1 + e^{y_j}) = f_\omega(\mathbf{y}) \frac{e^{y_i}}{1 + e^{y_i}}.$$

Therefore, if $\mathbf{y} \to \gamma$ is the transformation defined as $\gamma = (\gamma_1, \ldots, \gamma_d)^t$, with $\gamma_i := \frac{e^{y_i}}{1+e^{y_i}}$, then

$$\nabla f_\omega(\mathbf{y}) = f_\omega(\mathbf{y})\,\gamma,$$

which implies that $\nabla f_\omega(\mathbf{y}) \neq 0$, for all $\mathbf{y} \in \mathbb{R}^d$. In particular, if $\nabla f_\omega(\mathbf{y})$ is not orthogonal to F, a small perturbation in the direction of the projection of $\nabla f_\omega(\mathbf{y})$ onto F will increase f_ω. This shows the first statement in the lemma.

On the other hand:

$$\frac{\partial^2 f_\omega}{\partial y_i^2}(\mathbf{y}) = e^{y_i} \prod_{j \neq i} (1 + e^{y_j}) = f_\omega(\mathbf{y})\,\gamma_i,$$

and for $i \neq j$:

$$\frac{\partial^2 f_\omega}{\partial y_j y_i}(\mathbf{y}) = e^{y_i} e^{y_j} \prod_{k \neq i,j} (1 + e^{y_k}) = f_\omega(\mathbf{y})\,\gamma_i \gamma_j.$$

As a result, $\nabla^2 f_\omega(\mathbf{y})$, the Hessian matrix of f_ω at $\mathbf{y}$, admits the decomposition:

$$\nabla^2 f_\omega(\mathbf{y}) = f_\omega(\mathbf{y})\,\big(\Gamma_1 + \Gamma_2\big),$$

where $\Gamma_1 := \mathrm{diag}\big(\gamma_1(1-\gamma_1), \ldots, \gamma_d(1-\gamma_d)\big)$, and

$$\Gamma_2 := \begin{bmatrix} \gamma_1^2 & \gamma_1\gamma_2 & \cdots & \gamma_1\gamma_d \\ \gamma_2\gamma_1 & \gamma_2^2 & \cdots & \gamma_2\gamma_d \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_d\gamma_1 & \gamma_d\gamma_2 & \cdots & \gamma_d^2 \end{bmatrix} = \gamma\gamma^t.$$

Because each $0 < \gamma_i < 1$, Γ_1 is strictly positive definite. Since Γ_2 is positive semidefinite, and $f_\omega(\mathbf{y}) > 0$ for all $\mathbf{y} \in \mathbb{R}^d$, $\nabla^2 f_\omega(\mathbf{y})$ is strictly positive definite regardless of $\mathbf{y}$. As a result, if $\nabla f_\omega(\hat{\mathbf{y}})$ is orthogonal to F, then $\hat{\mathbf{y}}$ is a local minimum of f_ω along F. This completes the proof of the lemma. ◀

Finally, combining Corollary 6 and Lemma 7, we obtain the following central result, which implies that the maxima in (13) can occur only occur among a finite number of well-characterized points in $\tilde{\mathcal{Q}}_\omega$.

▶ **Theorem 8.** *If $P > 0$ then, for each $\omega \in \{0,1\}^d$, the maximum $\max_{\mathbf{y} \in \tilde{\mathcal{Q}}_\omega} f_\omega(\mathbf{y})$, can only occur at a vertex of $\tilde{\mathcal{Q}}_\omega$.*

3 Algorithms for $\lambda(P)$

Computing $\lambda(P)$ requires solving the optimization problem (13) for each of 2^d possible binary outcomes. As previously described, solving each optimization problem can be achieved by evaluating f_ω at each vertex of $\tilde{\mathcal{Q}}_\omega$, and the vertices can be found as unique solutions of invertible $(d \times d)$-subsystems $A'_\omega \mathbf{y} = \mathbf{b}'_\omega$. This motivates Algorithm 1, which computes $\lambda(P)$ by exploring square subsystems of $A_\omega \mathbf{y} \leq \mathbf{b}_\omega$ to find vertices, evaluating $f_\omega(\mathbf{y}^*)$ at each vertex $\mathbf{y}^*$ for each outcome ω, and returning the largest of these.

For each outcome ω, there are $\binom{2^d-1}{d}$ subsystems $A'_\omega \mathbf{y} = \mathbf{b}'_\omega$ of size $(d \times d)$ to check. For each subsystem $A'_\omega \mathbf{y} = \mathbf{b}'_\omega$, simple Gaussian elimination will find a unique solution, if it exists, in $O(d^3)$ time, and often terminates in less time if A'_ω is singular. If $\mathbf{y}'$ is a

Algorithm 1 A naïve exact algorithm for $\lambda(P)$.

Require: $P > 0$
  $M \leftarrow 0$
  for $\omega \in \{0,1\}^d$ **do**
    $A_\omega \leftarrow \{[\![\omega_i \neq \nu_i]\!]_{i=1,\ldots,d}\}_{\nu\in\{0,1\}^d\setminus\{\omega\}}$
    $\mathbf{b}_\omega \leftarrow \{\log(\frac{P(\nu)}{P(\omega)})\}_{\nu\in\{0,1\}^d\setminus\{\omega\}}$
    for $\{\nu^{(1)}, \nu^{(2)}, \ldots, \nu^{(d)}\} \subset \{0,1\}^d \setminus \{\omega\}$ **do**
      $A'_\omega \leftarrow \{[\![\omega_i \neq \nu_i^{(j)}]\!]\}_{i,j=1,\ldots,d}$
      $\mathbf{b}'_\omega \leftarrow \{\log(\frac{P(\nu^{(j)})}{P(\omega)})\}_{j=1,\ldots,d}$
      if A'_ω is invertible **then**
        $\mathbf{y}^* \leftarrow (A'_\omega)^{-1}\mathbf{b}'_\omega$
        if $A_\omega \mathbf{y}^* \leq \mathbf{b}_\omega$ **then**
          $M \leftarrow M \vee f_\omega(\mathbf{y}^*)$
  return $\lambda(P) \leftarrow M$

unique solution to the square subsystem $A'_\omega \mathbf{y}' = \mathbf{b}'_\omega$, it takes $O(d2^d)$ operations to check that $\mathbf{y}'$ is feasible, i.e., $A_\omega \mathbf{y}' \leq \mathbf{b}_\omega$. If $\mathbf{y}'$ is infeasible, it often takes many fewer operations to confirm this.

Taking these operations together, and using the well-known bound on binomial coefficients, $\binom{n}{k} < (\frac{n\cdot e}{k})^k$, in the worst case there are $O\left(d^4(\frac{2^{d+1}e}{d})^d\right)$ operations required to compute $\lambda(P)$. The memory required by this algorithm grows much less slowly, as $O(2^d)$, if square subsystems are iterated without loading every set of d indices into memory. This is common in standard combinatorial software like the `itertools` module in Python [4, Section 3.2]. In practice, we find that without any parallelization strategies and without supercomputing resources, it is feasible to compute $\lambda(P)$ for binary sources up to dimension $d = 6$ by naïvely searching for vertices.

We note that specialized algorithms to explore only those subsystems $A'_\omega \mathbf{y} = \mathbf{b}'_\omega$ which are invertible, and ignore singular subsystems, are still unlikely to allow computation of $\lambda(P)$ in very high dimensions. In fact, the number of invertible submatrices A'_ω of dimension d has previously been recognized as a noteworthy sequence [3]. This sequence is hard to compute explicitly, but appears to grow exponentially fast. In fact, there are approximately 2.52×10^{14} invertible subsystems in only 8 binary dimensions [12].

Specialized polyhedral programming algorithms may help to accelerate computation of $\lambda(P)$. For example, the vertex enumeration algorithm given in [1], runs in $O(d2^dV)$ time, where V is the number of vertices of $\tilde{\mathcal{Q}}_\omega$. The number of vertices is hard to characterize (it depends on $\mathbf{b}_\omega$), but based on simulation we believe it is typically much smaller than the number of invertible subsystems. We believe a pivoting method similar to [1] can be adapted to take advantage of A_ω's binary structure.

Some readers may note that each optimization program:

$$\begin{aligned} \max_{\mathbf{y}\in\mathbb{R}^d} \quad & f_\omega(\mathbf{y}) \\ \text{subject to} \quad & A_\omega \mathbf{y} \leq \mathbf{b}_\omega \end{aligned}$$

resembles a linear program. However, the objective function $f_\omega(\mathbf{y})$ is nonlinear, and therefore linear programming techniques such as Dantzig's simplex algorithm [2, Chapter 5] are not suitable. Moreover, positive definiteness of the Hessian derived in Lemma 7 implies that $f_\omega(\mathbf{y})$ is strictly convex. Although the feasible region is also convex, the fact that we seek to *maximize* $f_\omega(\mathbf{y})$ means most nonlinear convex programming techniques cannot be guaranteed to converge to true maxima.

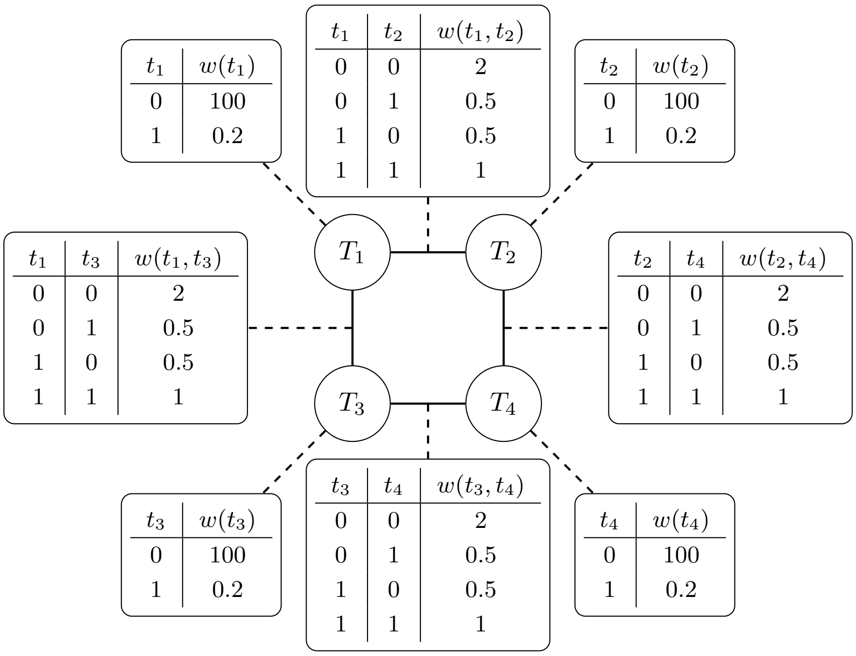

Figure 2 Markov network that models the interaction of four hypothetical patients that may or may not have tuberculosis. Patient i is healthy if $T_i = 0$, and infected if $T_i = 1$.

Due to the aforementioned difficulties in the combinatorial approach in high dimensions, we have also explored numerical approximation of each optimization program using nonlinear algorithms including sequential gradient-free linear approximation (COBYLA) [9], and sequential quadratic programming (SLSQP) [6]. These show some promise but tend to suffer from numerical instability in moderate to high dimensions (above $d = 5$ or so). However, because the structure of f_ω makes computing higher-order derivatives very straightforward, it may be possible to devise a specialized interior point method that makes approximating $\lambda(P)$ efficient even in higher dimensions.

4 Proof of Concept

Consider the Markov network [5] in Figure 2, borrowed from [11, Chapter 2]. In this setting, undirected edges represent interactions in a social network of four patients, each of whom may or may not have tuberculosis (represented as four Bernoulli random variables $T_1, \ldots, T_4$). Here, the complete subgraphs (cliques) of the Markov network are $\{T_1\}, \{T_2\}, \{T_3\}, \{T_4\}, \{T_1, T_2\}, \{T_1, T_3\}, \{T_2, T_4\}$, and $\{T_3, T_4\}$. To each clique C we associate a *factor* $w : \{0,1\}^{|C|} \to \mathbb{R}_+$, and to each configuration $(t_1, t_2, t_3, t_4) \in \{0,1\}^4$ of sick and healthy patients, we associate the probability:

$$P(t_1, t_2, t_3, t_4) \propto w(t_1) \cdot w(t_2) \cdot w(t_3) \cdot w(t_4) \cdot w(t_1, t_2) \cdot w(t_1, t_3) \cdot w(t_2, t_4) \cdot w(t_3, t_4).$$

This network reflects the intuition that, if one patient who has tuberculosis interacts with another, it is more likely for the latter to have tuberculosis. In fact, the joint distribution P of (T_1, T_2, T_3, T_4) is *exchangeable* (i.e. labels on the patients can be permuted without affecting the joint probability of their tuberculosis status). Using Algorithm 1, we find that $\lambda(P)$ is very close to one. We transform a vertex y^* which achieves $\lambda(P)$ back to a probability q^* (see Corollary 3) and find explicitly:

$$P = 0.999999 \cdot Be(0.000125) \otimes Be(0.000125) \otimes Be(0.000125) \otimes Be(0.000125) + 0.0000001 \cdot R,$$

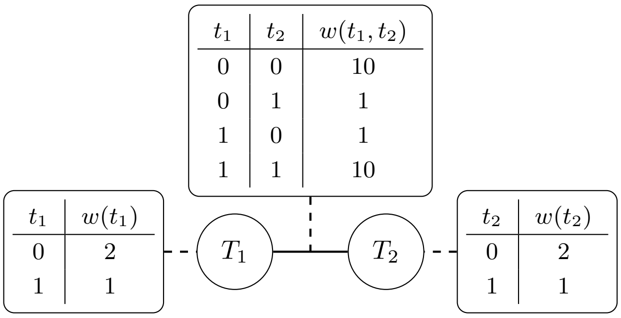

Figure 3 Markov network that models the interaction of two hypothetical patients which may or may not have tuberculosis. In this setting, the marginal probability of a patient being infected with tuberculosis is moderate ($\approx 22\%$), and the probability that exactly one of the two patients is infected is relatively low ($\approx 8\%$). This might be a realistic model for, e.g., two inmates sharing a cell in a prison with a tuberculosis outbreak.

where R is a residual probability distribution with low entropy (≈ 2 bits, compared to the uniform distribution over $\{0, 1\}^4$, which has 4 bits of entropy). This means that, despite the dependence implied by the interactions, a large fraction of the time it will appear as though the patients are infected with tuberculosis independently, each with a very small probability of infection.

It is not always the case that a source represented by a probabilistic graphical model has a very large independent weight. Consider a simpler version of the previous Markov network, shown in Figure 3. In this case, a non-negligible fraction of the data produced by the source cannot be recapitulated by a model with independent marginal distributions. Let P denote the joint distribution of (T_1, T_2). Using Algorithm 1, we find that $\lambda(P) = 0.817$. Moreover,

$$P = 0.817 \cdot Be(0.048) \otimes Be(0.048) + 0.183 \cdot \delta_{(1,1)}.$$

That is, a large fraction of the time a realization of these two patients' tuberculosis states cannot be attributed to the largest independent component of P.

These two examples demonstrate how scientists and engineers may benefit from detecting a source's independent weight. If a source under study is known to have $\lambda(P) \approx 1$, even if the source fails a hypothesis test of independence, the modeler might save considerable complexity while still recapitulating most of the features of the source. In contrast, if a source has very low independent weight, the scientist could find meaningful mechanistic insights in the residual component, such as in the latter example, where a sample originates *either* from a hidden non-degenerate probability model with independent marginals or a deterministic one.

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Block Statistics in Subcritical Graph Classes

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Abstract

We study block statistics in subcritical graph classes; these are statistics that can be defined as the sum of a certain weight function over all blocks. Examples include the number of edges, the number of blocks, and the logarithm of the number of spanning trees. The main result of this paper is a central limit theorem for statistics of this kind under fairly mild technical assumptions.

2012 ACM Subject Classification Mathematics of computing → Random graphs; Mathematics of computing → Generating functions

Keywords and phrases subcritical graph class, block statistic, number of blocks, number of edges, number of spanning trees

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.24

Funding *Dimbinaina Ralaivaosaona*: Supported by Division for Research Development (DRD) of Stellenbosch University and the National Research Foundation (NRF) of South Africa.
Clément Requilé: Supported by the Special Research Program F50 *Algorithmic and Enumerative Combinatorics* of the Austrian Science Fund.
Stephan Wagner: Supported by the Knut and Alice Wallenberg Foundation.

1 Introduction

The detailed analytic study of *subcritical graph classes* was initiated by Drmota et al. in their seminal paper [4]; the formal definition, which will be given below, is based on properties of the generating function. Intuitively speaking, subcritical classes are "tree-like" in some sense, which is exhibited for instance by the fact that their scaling limit is the continuum random tree [12], meaning that the global structure is essentially determined by the block-cutpoint tree, while the blocks themselves are fairly small. Typical examples of subcritical graph classes are trees, cacti, block graphs, outerplanar graphs and series-parallel graphs. Unfortunately, there is probably no simple graph-theoretical characterisation of subcritical graph classes, as it was shown that every proper minor-closed family of graphs is contained in a subcritical family [9].

By a block statistic, we mean an invariant induced by a weight function w on all 2-connected graphs (blocks) of the specific graph class. Any graph G can be decomposed uniquely into maximal 2-connected subgraphs $B_1, B_2, \dots, B_k$ (that can only be joined at cutvertices), the so-called blocks of G. Using this decomposition, we define the block statistic S_w associated with w by

$$S_w(G) = \sum_{j=1}^{k} w(B_j).$$

31st International Conference on Probabilistic, Combinatorial and Asymptotic Methods for the Analysis of Algorithms (AofA 2020).
Editors: Michael Drmota and Clemens Heuberger; Article No. 24; pp. 24:1–24:14
Leibniz International Proceedings in Informatics
LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

Let us give a few motivating examples of block statistics:

- The trivial weight function defined by $w(B) = 1$ for all possible blocks B yields the number of blocks.
- If we fix some block A and define

  $$w_A(B) = \begin{cases} 1 & B \simeq A, \\ 0 & \text{otherwise}, \end{cases}$$

  the associated block statistic is the number of (isomorphic) occurrences of A as a block.
- If the weight function $w(B)$ is the number of edges in B, then the associated block statistic $S_w(G)$ gives the number of edges of G.
- Let $\tau(B)$ be the number of spanning trees of a block B, and set $w(B) = \log \tau(B)$. Since every spanning tree of a connected graph decomposes uniquely into spanning trees on all the blocks, we have

  $$\tau(G) = \prod_{j=1}^{k} \tau(B_j)$$

  if $B_1, B_2, \ldots, B_k$ are the blocks of a connected graph G. This translates to

  $$S_w(G) = \log \tau(G).$$
- Since the Tutte polynomial is also multiplicative over blocks, the previous example generalises to many others that are special values of the Tutte polynomial, specifically the (logarithm of the) number of subforests, spanning forests, connected spanning subgraphs, acyclic orientations and strongly connected orientations.
- The number of nontrivial complete subgraphs (i.e., complete subgraphs with more than one vertex) is also a block statistic in our sense, since every such subgraph needs to be contained entirely in one of the blocks.
- The number of occurrences of a fixed graph H as an induced subgraph, which was studied in [6], is not always a block statistic (since a copy of H may involve vertices of several blocks), but it becomes one if H is 2-connected.

The number of blocks and the number of edges were already shown by Drmota et al. [4] to satisfy a central limit theorem, the latter under the assumption (that was satisfied for all the examples studied in their paper) that the graphs are planar, so that the number of edges is necessarily linear in the number of vertices. However, this is not satisfied for all subcritical classes of graphs (block graphs, for example, are an exception), and there are also other statistics among the aforementioned for which the weight function can grow faster than linearly in the block size, for example the logarithm of the number of spanning trees, for which the weight can be as large as $w(B) = (|B| - 2) \log |B|$ when B is a complete graph. We are therefore interested in proving central limit theorems under weaker assumptions on the growth of the weights.

Before we formulate our main results, let us recall the formal definition of a subcritical graph class. For simplicity, we will restrict ourselves to the labelled case.

► **Definition 1.** *We call a class of graphs $\mathcal{G}$* block-stable *if it has the property that a graph G belongs to $\mathcal{G}$ if and only if each of its blocks belongs to $\mathcal{G}$. Now let $\mathcal{G}$ be a block-stable class of labelled graphs, and denote the subclasses of connected graphs and 2-connected graphs in $\mathcal{G}$ by $\mathcal{C}$ and $\mathcal{B}$ respectively. Since every graph can be seen as the union of its connected components, we have the symbolic decomposition*

$$\mathcal{G} = \mathrm{Set}(\mathcal{C}).$$

More importantly (for the definition of subcriticality), rooted connected graphs (indicated by $\mathcal{C}^\bullet$) can be decomposed as follows:

$$\mathcal{C}^\bullet = \mathcal{Z} \times \mathrm{Set}(\mathcal{B}' \circ \mathcal{C}^\bullet),$$

where $\mathcal{Z}$ stands for a single vertex, and $\mathcal{B}'$ for the class derived from $\mathcal{B}$ by not labelling one of the vertices. In words: a rooted connected graph decomposes into the root, the set of blocks that contain the root, and rooted connected graphs attached to all non-root vertices of the root blocks.

On the level of generating functions $G(z)$, $C(z)$ and $B(z)$ are associated with $\mathcal{G}$, $\mathcal{C}$ and $\mathcal{B}$ respectively, this yields

$$G(z) = \exp(C(z)) \tag{1}$$

and

$$C^\bullet(z) = z\exp(B'(C^\bullet(z)), \tag{2}$$

where $C^\bullet(z) = zC'(z)$ is the generating function for $\mathcal{C}^\bullet$. The class $\mathcal{G}$ is now said to be subcritical *if the radii of convergence ρ and η of C and B satisfy the inequality*

$$\gamma = C^\bullet(\rho) < \eta. \tag{3}$$

As it was shown in [4], the generating function $C^\bullet$ has a square root singularity for every subcritical class, which allows us to apply singularity analysis to derive asymptotic formulas for counting graphs of given order in $\mathcal{G}$ or $\mathcal{C}$.

▶ **Theorem 2** ([4]). *For every subcritical family of graphs, the generating function $C^\bullet$ is analytic in a region of the form*

$$\{z \in \mathbb{C} : |z| < r, |\operatorname{Arg}(z-\rho)| > \phi\}$$

for some $r > \rho$ and $\phi \in (0, \frac{\pi}{2})$. At the singularity ρ, it has an asymptotic expansion of the form

$$C^\bullet(z) = \gamma + \gamma_1(1-z/\rho)^{1/2} + \gamma_2(1-z/\rho) + \gamma_3(1-z/\rho)^{3/2} + O((1-z/\rho)^2). \tag{4}$$

Here, $\gamma > 0$ is the unique positive solution of the equation $\gamma B''(\gamma) = 1$, and $\rho = \gamma\exp(-B'(\gamma))$.

It is sometimes useful to have explicit expressions for γ_1 and γ_2. They are given by

$$\gamma_1 = -\sqrt{\frac{2\gamma^2}{1+\gamma^2 B'''(\gamma)}} \quad \text{and} \quad \gamma_2 = \frac{2\gamma - \gamma^4 B''''(\gamma)}{3(1+\gamma^2 B'''(\gamma))^2},$$

respectively, as one can see e.g. by comparing coefficients on the two sides of the functional equation (and using the identity $\gamma B''(\gamma) = 1$ to simplify).

2 The generating function for a block statistic

The functional equations (1) and (2) can be modified in a straightforward fashion to include the block statistic S_w. Let us define the bivariate function

$$C(z,t) = \sum_{C \in \mathcal{C}} \frac{z^{|C|}}{|C|!} e^{S_w(C)t},$$

and $G(z,t)$ in an analogous fashion. To keep notation simple, we do not indicate the dependence of the generating functions on w. Since S_w is additive over connected components, we clearly have

$$G(z,t) = \exp(C(z,t)).$$

Moreover, if we set

$$B(z,t) = \sum_{B \in \mathcal{B}} \frac{z^{|B|}}{|B|!} e^{w(B)t},$$

then (2) changes to

$$C^\bullet(z,t) = z \exp\big(B_z(C^\bullet(z,t),t)\big), \tag{5}$$

where B_z is the partial derivative with respect to z. Of course, when $t = 0$, everything simplifies to (1) and (2). It is important to notice that the sum defining B might not be convergent: if $w(B)$ has faster than linear growth for at least some blocks B, then the radius of convergence in z can become zero for all $t > 0$. Therefore, B and C are a priori only regarded as formal power series.

If, however, $w(B) = O(|B|)$, then the radius of convergence of B as a function of t changes continuously, so if t is close enough to zero, the inequality that defines a subcritical class remains true, and $C^\bullet$ still has a square root singularity, the position of which moves continuously with t. We are therefore in the scheme of [3, Theorems 2.21–2.23], and the quasi-power theorem ([10], see also [8, Section IX.5]) yields a central limit theorem almost automatically. This was in fact exploited in [4] to obtain the central limit theorems for number of edges and number of blocks.

However, not all interesting block statistics satisfy the condition $w(B) = O(|B|)$. The example of the logarithm of the number of spanning trees was mentioned earlier; others include the logarithm of the number of subforests, spanning forests or connected spanning subgraphs and the number of nontrivial complete subgraphs. Thus, we follow a slightly different route imposing somewhat milder conditions on the weight function w. Specifically, we will prove the following theorem:

▶ **Theorem 3.** *Consider a subcritical class of graphs with a weight function w on the blocks. Let W_n be the average of $w(B)^2$ over all blocks B on n vertices. Suppose that*

$$\limsup_{n\to\infty} W_n^{1/n} < \frac{\eta}{\gamma}, \tag{6}$$

with γ and η as in (3). Let C_n denote a random connected graph with n vertices in our subcritical class of graphs. The following statements on the distribution of $S_w(C_n)$ hold:

1. *There exist constants μ and λ such that the mean $\mathbb{E}(S_w(C_n))$ is asymptotically equal to $\mu n - \lambda + O(n^{-1})$.*
2. *There exists a constant $\sigma^2 \geq 0$ such that the variance $\mathbb{V}(S_w(C_n))$ is asymptotically equal to $\sigma^2 n + O(1)$. Moreover, we have $\sigma^2 > 0$ unless the weight function w is of the form $w(B) = c(|B| - 1)$ for some constant c.*
3. *If $\sigma^2 > 0$, then the distribution of $S_w(C_n)$ converges, suitably normalised by subtracting the mean and dividing by the standard deviation, weakly to a standard normal distribution.*

Intuitively, (6) states that the block generating function, with blocks weighted by $w(B)^2$, still satisfies the subcriticality condition. Most of the examples mentioned in the introduction satisfy the conditions of the theorem for all subcritical classes, since the growth of the weight function w is subexponential. Notable examples include the number of blocks, the number of edges and the (logarithm of the) number of spanning trees. It is possible that the condition is satisfied even if the weight grows exponentially in the block size, though. Importantly, blocks in random graphs from a subcritical class are typically small (the largest block only being logarithmic in size). This makes it possible that $\mathbb{E}(S_w(C_n))$ is linear in n even in cases where w can grow exponentially.

▶ Remark 4. While we are focusing on connected graphs in this paper, it would also be possible to transfer our results to arbitrary random graphs from the specific subcritical class of graphs.

▶ Remark 5. We remark that $S_w(C) = c(|C|-1)$ holds deterministically for all connected graphs C in the "degenerate" case that $w(B) = c(|B|-1)$, so that the variance is identically 0.

Several explicit examples are presented in detail in the appendix. The following table gives an overview:

Graph class	Block statistic	μ	σ^2	Sect.
Cacti	Number of blocks	0.64780	0.21218	A.1
	Number of edges	1.19149	0.06272	A.1
	Number of spanning trees (log)	0.24985	0.08007	A.1
	Number of connected spanning subgraphs (log)	0.29690	0.12113	A.1
Block graphs	Number of blocks	0.76322	0.12512	A.2
	Number of edges	1.28357	0.31267	A.2
	Number of spanning trees (log)	0.28580	0.23671	A.2
	Number of nontrivial complete subgraphs	1.69146	4.55177	A.2
Series-parallel graphs	Number of blocks	0.14937	0.14875	A.3
	Number of edges	1.61673	0.21125	A.3
	Number of spanning trees (log)	??	??	A.3

In the last example, numerical values of μ and σ^2 are surprisingly difficult to determine. This will be explained in Section A.3.

3 Mean and variance

It is somewhat easier for our calculations to consider rooted graphs. However, since every labelled graph with n vertices corresponds to precisely n rooted graphs, all distributional results that we obtain for rooted graphs in the following hold automatically for unrooted graphs as well.

In order to obtain asymptotic formulas for mean and variance, we consider the partial derivatives of $C^\bullet(z,t)$ with respect to t at $t=0$. Differentiating (5) with respect to t yields

$$\begin{aligned} C_t^\bullet(z,t) &= z\exp\big(B_z(C^\bullet(z,t),t)\big)\Big(B_{zz}(C^\bullet(z,t),t)C_t^\bullet(z,t) + B_{zt}(C^\bullet(z,t),t)\Big) \\ &= C^\bullet(z,t)\Big(B_{zz}(C^\bullet(z,t),t)C_t^\bullet(z,t) + B_{zt}(C^\bullet(z,t),t)\Big). \end{aligned}$$

We solve for $C_t^\bullet(z,t)$, which gives us

$$C_t^\bullet(z,t) = \frac{C^\bullet(z,t)B_{zt}(C^\bullet(z,t),t)}{1 - C^\bullet(z,t)B_{zz}(C^\bullet(z,t),t)}.$$

In the same way, we can also differentiate with respect to z, which yields

$$C^\bullet_z(z,t) = \frac{C^\bullet(z,t)}{z(1 - C^\bullet(z,t)B_{zz}(C^\bullet(z,t),t))}.$$

Thus we have

$$C^\bullet_t(z,t) = zC^\bullet_z(z,t)B_{zt}(C^\bullet(z,t),t). \tag{7}$$

The second derivative is determined in a similar fashion. Differentiating (7) with respect to z and t respectively (and plugging in $t = 0$), we obtain

$$C^\bullet_{zt}(z,0) = C^\bullet_z(z,0)B_{zt}(C^\bullet(z,0),0) + zC^\bullet_{zz}(z,0)B_{zt}(C^\bullet(z,0),0) + zC^\bullet_z(z,0)^2B_{zzt}(C^\bullet(z,0),0)$$

and

$$\begin{aligned} C^\bullet_{tt}(z,0) &= zC^\bullet_{zt}(z,0)B_{zt}(C^\bullet(z,0),0) + zC^\bullet_z(z,0)C^\bullet_t(z,0)B_{zzt}(C^\bullet(z,0),0) \\ &\quad + zC^\bullet_z(z,0)B_{ztt}(C^\bullet(z,0),0). \end{aligned}$$

We plug the former equation into the latter, and also replace $C^\bullet_t(z,0)$ by the equation given in (7) to arrive at the following representation for $C^\bullet_{tt}(z,0)$:

$$\begin{aligned} C^\bullet_{tt}(z,0) &= z^2C^\bullet_{zz}(z,0)B_{zt}(C^\bullet(z,0),0)^2 + 2z^2C^\bullet_z(z,0)^2B_{zt}(C^\bullet(z,0),0)B_{zzt}(C^\bullet(z,0),0) \\ &\quad + zC^\bullet_z(z,0)\big(B_{zt}(C^\bullet(z,0),0)^2 + B_{ztt}(C^\bullet(z,0),0)\big). \end{aligned} \tag{8}$$

Note that this representation, like (7), only involves derivatives of $C^\bullet(z,t)$ with respect to z, so that we can use our knowledge of the behaviour of $C^\bullet(z,0)$ given in Theorem 2.

▶ **Theorem 6.** *Under the conditions stated in Theorem 3, the mean of the block statistic S_w over all graphs in $\mathcal{C}$ with n vertices is asymptotically*

$$\mathbb{E}(S_w(C_n)) = \mu n - \lambda + O(n^{-1}),$$

with $\mu = B_{zt}(\gamma,0)$ and

$$\lambda = \frac{3\gamma_2}{2}B_{zzt}(\gamma,0) + \frac{\gamma_1^2}{4}B_{zzzt}(\gamma,0).$$

Proof. Note that

$$B_{tt}(z,0) = \sum_{n\ge 2}\Big(\sum_{\substack{B\in\mathcal{B}\\|B|=n}} w(B)^2\Big)\frac{z^n}{n!} = \sum_{n\ge 2} W_nB_n\frac{z^n}{n!},$$

where B_n is the number of blocks with n labelled vertices. The radius of convergence of $B(z,0)$ is $\eta = 1/\limsup_{n\to\infty}(B_n/n!)^{1/n}$, since the coefficient of z^n in $B(z,0)$ is $B_n/n!$. The technical condition (6) has been chosen in such a way that the radius of convergence of $B_{tt}(z,0)$, which is

$$\begin{aligned} \frac{1}{\limsup_{n\to\infty}(W_nB_n/n!)^{1/n}} &> \frac{1}{\limsup_{n\to\infty} W_n^{1/n}} \cdot \frac{1}{\limsup_{n\to\infty}(B_n/n!)^{1/n}} \\ &= \frac{\eta}{\limsup_{n\to\infty} W_n^{1/n}}, \end{aligned}$$

is greater than γ. The radius of convergence of $B(z,0)$ is $\eta > \gamma$ by the definition of subcriticality, and the Cauchy-Schwarz inequality implies that

$$|B_t(z,0)|^2 = \Big| \sum_{B\in\mathcal{B}} \frac{z^{|B|}w(B)}{|B|!} \Big|^2 \le \sum_{B\in\mathcal{B}} \frac{|z|^{|B|}w(B)^2}{|B|!} \sum_{B\in\mathcal{B}} \frac{|z|^{|B|}}{|B|!} = B_{tt}(|z|,0)B(|z|,0).$$

This shows that $B_t(z,0)$ also has greater radius of convergence than γ. Thus $B_t(z,0)$, $B_{tt}(z,0)$ and all their derivatives with respect to z are analytic in a disk around 0 that includes γ. Now since $C^\bullet$ is amenable to singularity analysis, so is

$$C_t^\bullet(z,0) = zC_z^\bullet(z,0)B_{zt}(C^\bullet(z,0),0).$$

In particular, this function and other partial derivatives of $C^\bullet$ that we consider have a Puiseux expansion around the singularity ρ whose exponents are integers or half-integers. Specifically, in view of (4), we have

$$\begin{aligned} B_{zt}(C^\bullet(z,0),0) &= B_{zt}(\gamma,0) + B_{zzt}(\gamma,0)(C^\bullet(z,0)-\gamma) + \frac{B_{zzzt}(\gamma,0)}{2}(C^\bullet(z,0)-\gamma)^2 \\ &\quad + O\big((C^\bullet(z,0)-\gamma)^3\big) \\ &= B_{zt}(\gamma,0) + \gamma_1 B_{zzt}(\gamma,0)(1-z/\rho)^{1/2} \\ &\quad + \Big(\gamma_2 B_{zzt}(\gamma,0) + \frac{\gamma_1^2 B_{zzzt}(\gamma,0)}{2}\Big)(1-z/\rho) + O\big((1-z/\rho)^{3/2}\big). \end{aligned}$$

Thus we can represent $C_t^\bullet(z,0)$ as follows:

$$C_t^\bullet(z,0) = B_{zt}(\gamma,0)zC_z^\bullet(z,0) + \kappa_1 - \Big(\frac{3\gamma_2 B_{zzt}(\gamma,0)}{2} + \frac{\gamma_1^2 B_{zzzt}(\gamma,0)}{4}\Big)C^\bullet(z,0) + O\big(1-z/\rho\big)$$

for some constant κ_1. It would be possible to add further terms to the expansion. By the principles of singularity analysis, we obtain

$$[z^n]C_t^\bullet(z,0) = \mu[z^n]zC_z^\bullet(z,0) - \lambda[z^n]C^\bullet(z,0) + O(n^{-1}[z^n]C^\bullet(z,0))$$

with μ and λ as given in the statement of the theorem. Therefore,

$$\mathbb{E}(S_w(C_n)) = \frac{[z^n]C_t^\bullet(z,0)}{[z^n]C^\bullet(z,0)} = \mu n - \lambda + O(n^{-1}). \qquad \blacktriangleleft$$

▶ **Theorem 7.** *Under the conditions stated in Theorem 3, the variance of the block statistic S_w over all graphs in $\mathcal{C}$ with n vertices is asymptotically $\mathbb{V}(S_w(C_n)) = \sigma^2 n + O(1)$, with*

$$\sigma^2 = B_{ztt}(\gamma,0) - \frac{\gamma^2 B_{zzt}(\gamma,0)^2}{1+\gamma^2 B_{zzz}(\gamma,0)}.$$

If the weight w is not of the form $w(B) = c(|B|-1)$ (where c is constant), then σ^2 is strictly positive.

Proof. The asymptotic formula for the variance is derived in a similar fashion as the mean. We now need to consider the second derivative with respect to t as well. The expression for $C_{tt}^\bullet(z,0)$ in (8) can be expanded around the dominant singularity ρ in the same way as $C_t^\bullet(z,0)$. Without going through the full calculation, let us just give the final result stating that

$$C_{tt}^\bullet(z,0) = \mu^2\big(z^2C_{zz}^\bullet(z,0) + zC_z^\bullet(z,0)\big) + (\sigma^2 - 2\lambda\mu)zC_z^\bullet(z,0) + O(1)$$

around the singularity, with μ, λ, σ^2 as defined above. Again, it would be possible to improve on the error term by including further terms. Now we get

$$[z^n]C^{\bullet}_{tt}(z,0) = \big(\mu^2 n^2 + (\sigma^2 - 2\lambda\mu)n + O(1)\big)[z^n]C^{\bullet}(z,0).$$

This gives us the second moment of $S_w(C_n)$ as $\mu^2 n^2 + (\sigma^2 - 2\lambda\mu)n + O(1)$, and subtracting the square of the mean yields the stated asymptotic formula for the variance.

It remains to prove that $\sigma^2 \neq 0$ except for trivial cases where $S_w(C)$ depends on the number of vertices of C only. To this end, recall first that γ is determined by the equation

$$\gamma B''(\gamma) = \gamma B_{zz}(\gamma,0) = 1.$$

Thus we can rewrite the denominator in the expression for σ^2 as follows:

$$1 + \gamma^2 B_{zzz}(\gamma,0) = \gamma B_{zz}(\gamma,0) + \gamma^2 B_{zzz}(\gamma,0) = \sum_{B \in \mathcal{B}} \frac{(|B|-1)^2 \gamma^{|B|-1}}{(|B|-1)!}.$$

The remaining two terms in the expression are

$$B_{ztt}(\gamma,0) = \sum_{B \in \mathcal{B}} \frac{w(B)^2 \gamma^{|B|-1}}{(|B|-1)!}$$

and

$$\gamma^2 B_{zzt}(\gamma,0)^2 = \Big(\sum_{B \in \mathcal{B}} \frac{w(B)(|B|-1)\gamma^{|B|-1}}{(|B|-1)!}\Big)^2,$$

respectively. Thus

$$\sigma^2 = \sum_{B \in \mathcal{B}} \frac{w(B)^2 \gamma^{|B|-1}}{(|B|-1)!} - \frac{\Big(\sum_{B \in \mathcal{B}} \frac{w(B)(|B|-1)\gamma^{|B|-1}}{(|B|-1)!}\Big)^2}{\sum_{B \in \mathcal{B}} \frac{(|B|-1)^2 \gamma^{|B|-1}}{(|B|-1)!}}. \tag{9}$$

The Cauchy-Schwarz inequality immediately shows that $\sigma^2 > 0$ unless $w(B)$ is a constant multiple of $|B|-1$, in which case σ^2 is clearly 0. ◀

In order to illustrate the formulas for mean and variance, let us consider a concrete example that satisfies the conditions of Theorem 3 for all subcritical graph classes: the number of blocks. In this case, we have $B(z,t) = e^t B(z)$, which allows us to express μ and σ^2 in terms of B and γ only: the following formulas can also already been found in [4].

$$\mu = B'(\gamma) \quad \text{and} \quad \sigma^2 = B'(\gamma) - \frac{1}{1+\gamma^2 B'''(\gamma)}. \tag{10}$$

4 Limit distribution

Next we derive a general central limit theorem for the block statistic S_w. As a first step, we consider the case where w is finitely supported, i.e., where $w(B) = 0$ for all but finitely many blocks. In this case, $B(z,t)$ differs from $B(z)$ only in finitely many terms: letting $\mathcal{B}_0$ be the set of blocks for which $w(B) = 0$, we have

$$B(z,t) = \sum_{B \in \mathcal{B}} \frac{z^{|B|}}{|B|!} e^{w(B)t} = \sum_{B \in \mathcal{B} \setminus \mathcal{B}_0} \frac{z^{|B|}}{|B|!} e^{w(B)t} + \sum_{B \in \mathcal{B}_0} \frac{z^{|B|}}{|B|!} = B(z) + \sum_{B \in \mathcal{B} \setminus \mathcal{B}_0} \frac{z^{|B|}}{|B|!}(e^{w(B)t} - 1).$$

The sum over $\mathcal{B} \setminus \mathcal{B}_0$ is finite and thus represents a function that is entire in both z and t. We are therefore in a position to apply a general result on perturbations of functional equations: by [3, Theorem 2.21], there exists a positive constant $\delta > 0$ such that $C^\bullet(z,t)$ still has a dominant square root singularity for $|t| < \delta$:

$$C^\bullet(z) = \gamma(t) + \gamma_1(t)(1 - z/\rho(t))^{1/2} + O(1 - z/\rho(t)),$$

where $\rho(t)$ is analytic as a function of t for $|t| < \delta$. Singularity analysis gives us an asymptotic formula for the moment generating function of $S_w(C_n)$:

$$\mathbb{E}\big(e^{tS_w(C_n)}\big) = \frac{[z^n]C^\bullet(z,t)}{[z^n]C^\bullet(z,0)} = \frac{\gamma_1(t)}{\gamma_1}\Big(\frac{\rho}{\rho(t)}\Big)^n\big(1 + O(n^{-1})\big).$$

Thus we can apply the quasi-power theorem ([10], [8, Section IX.5]), which proves that $S_w(C_n)$ satisfies a central limit theorem in the case that w has finite support:

$$\frac{S_w(C_n) - \mathbb{E}(S_w(C_n))}{\sqrt{\mathbb{V}(S_w(C_n))}} \xrightarrow{\mathrm{d}} N(0,1).$$

This line of reasoning does not apply if w grows too fast; with the weaker assumptions of Theorem 3, $C^\bullet(z,t)$ may no longer have a square root singularity for $t > 0$ (and might in fact have radius of convergence 0 as a power series in z). Therefore, we rather approximate S_w by considering truncated versions of the weight function w.

For a positive integer M, set

$$w^{(M)}(B) = \begin{cases} w(B) & \text{if } |B| \le M, \\ 0 & \text{otherwise.} \end{cases}$$

We observe that $w^{(M)}$ has finite support, so the block statistic $S_w^{(M)}$ associated with $w^{(M)}$ satisfies a central limit theorem as stated above. Clearly, every block statistic with finitely supported weight function satisfies the conditions of Theorem 3, thus in particular the statements on mean and variance in Theorem 6 and Theorem 7 apply:

- $\mathbb{E}(S_w^{(M)}(C_n)) = \mu_M n + O(1)$,
- $\mathbb{V}(S_w^{(M)}(C_n)) = \sigma_M^2 n + O(1)$,
- $\frac{S_w^{(M)}(C_n) - \mu_M n}{\sigma_M\sqrt{n}} \xrightarrow{\mathrm{d}} N(0,1)$, or equivalently $\frac{S_w^{(M)}(C_n) - \mathbb{E}(S_w^{(M)}(C_n))}{\sqrt{n}} \xrightarrow{\mathrm{d}} N(0,\sigma_M^2)$.

We can now apply the following lemma (see for instance [11, Theorem 4.28]):

▶ **Lemma 8.** *Let $(X_n)_{n\ge1}$ and $(W_{N,n})_{N,n\ge1}$ be sequences of random variables with mean 0. Assume that for some random variables W_N $(N \ge 1)$ and W, we have*

- *$W_{N,n} \xrightarrow{\mathrm{d}} W_N$ as $n \to \infty$ for every $N \ge 1$, and $W_N \xrightarrow{\mathrm{d}} W$ as $N \to \infty$.*
- *$\mathbb{V}(X_n - W_{N,n}) \le C_N$ for some constants C_N uniformly in n, and $C_N \to 0$ as $N \to \infty$.*

Then we also have $X_n \xrightarrow{\mathrm{d}} W$ as $n \to \infty$.

In our setting, we take

$$X_n = \frac{S_w(C_n) - \mathbb{E}(S_w(C_n))}{\sqrt{n}} \quad \text{and} \quad W_{N,n} = \frac{S_w^{(N)}(C_n) - \mathbb{E}(S_w^{(N)}(C_n))}{\sqrt{n}}.$$

Note that these random variables all have mean 0. Since the sums in the formula (9) for σ^2 converge by our assumptions on the weight function w, the constants σ_N^2 converge: $\lim_{N\to\infty} \sigma_N^2 = \sigma^2$. So we have $W_{N,n} \xrightarrow{\mathrm{d}} W_N = N(0,\sigma_N^2)$ as $n \to \infty$ for every N, and $W_N \xrightarrow{\mathrm{d}} W = N(0,\sigma^2)$ as $N \to \infty$.

Lastly, the conditions of Theorem 3 also apply to $S_w(C_n) - S_w^{(N)}(C_n)$, which is the block statistic associated with the weight function that is given by

$$w(B) - w^{(N)}(B) = \begin{cases} 0 & \text{if } |B| \le N, \\ w(B) & \text{otherwise.} \end{cases}$$

Thus the formula of Theorem 7 applies, which yields

$$\begin{aligned} \mathbb{V}(X_n - W_{N,n}) &= \mathbb{V}\Big(\frac{S_w(C_n) - S_w^{(N)}(C_n) - \mathbb{E}(S_w(C_n) - S_w^{(N)}(C_n))}{\sqrt{n}} \Big) \\ &= \frac{1}{n} \mathbb{V}\big(S_w(C_n) - S_w^{(N)}(C_n)\big) = \tau_N^2 + O(n^{-1}) \end{aligned}$$

for some constants τ_N^2 that satisfy $\lim_{N\to\infty} \tau_N^2 = 0$. One can verify that the O-constant can be chosen to depend only on the graph class and the weight function w, but not on N. Moreover, we clearly have $X_n = W_{N,n}$ and thus $\mathbb{V}(X_n - W_{N,n}) = 0$ for $n \le N$. Thus all conditions of Lemma 8 are satisfied, and we obtain the desired central limit theorem for $S_w(C_n)$:

$$\frac{S_w(C_n) - \mathbb{E}(S_w(C_n))}{\sqrt{n}} \xrightarrow{\mathrm{d}} N(0, \sigma^2)$$

as $n \to \infty$. This finally completes the proof of Theorem 3.

5 Conclusion

We obtained a central limit theorem for block statistics under rather mild conditions that cover many natural cases. It would be interesting to see if there are natural examples where the conditions fail and there is no central limit theorem. There are also many examples of statistics that are not block statistics, but of a similar nature, for example the number of (arbitrary, maximal or maximum) independent sets or matchings, see [5] for some examples. One would still expect a log-normal limit law to hold in these cases, akin to spanning trees.

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A Examples

A.1 Cacti

Cacti are graphs whose blocks are either single edges or cycles. Thus there are $\frac{(n-1)!}{2}$ (labelled) blocks on n vertices for every $n > 2$, and precisely one block on two vertices. We find that the block generating function is given by

$$B(z) = \frac{z^2}{2} + \sum_{n=3}^{\infty} \frac{(n-1)!}{2n!} z^n = -\frac{1}{2}\log(1-z) + \frac{z^2}{4} - \frac{z}{2}.$$

One finds that γ is the positive root of the polynomial $z^3 - 4z^2 + 6z - 2$, and

$$\rho = \gamma \exp\big(-B'(\gamma)\big) = \gamma \exp\Big(-\frac{\gamma(2-\gamma)}{2(1-\gamma)}\Big).$$

Numerically, $\gamma \approx 0.45631$ and $\rho \approx 0.23874$. Let us now determine the modified generating function $B(z,t)$ for different choices of the weight function.

Number of blocks

In this case, we have $B(z,t) = e^t B(z)$, and we can apply the formulas in (10), which give us

$$\mu = B'(\gamma) \approx 0.64780 \quad \text{and} \quad \sigma^2 = B'(\gamma) - \frac{1}{1+\gamma^2 B'''(\gamma)} \approx 0.21218.$$

Number of edges

Here, $w(B) = |B|$ for all blocks B other than a single edge. Thus we have $B(z,t) = B(ze^t) + \frac{z^2}{2}(e^t - e^{2t})$. It is straightforward to determine numerical values for μ and σ^2 using this explicit formula for $B(z,t)$: we have $\mu \approx 1.19149$ and $\sigma^2 \approx 0.06272$.

Number of spanning trees and number of connected spanning subgraphs

For the number of spanning trees (more precisely, its logarithm), the appropriate weight function is given by $w(B) = \log|B|$ for $|B| > 2$, since a cycle of length k has precisely k spanning trees, and $w(B) = 0$ for $|B| = 2$. Thus

$$B(z,t) = \frac{z^2}{2} + \sum_{n=3}^{\infty} \frac{(n-1)!}{2n!} z^n e^{t\log n} = \frac{z^2}{2} + \frac{1}{2}\sum_{n=3}^{\infty} n^{t-1} z^n.$$

Thus the logarithm of the number of spanning trees in cacti is asymptotically normally distributed, with mean and variance asymptotically equal to μn and $\sigma^2 n$ respectively, where

$$\mu = B_{zt}(\gamma, 0) = \frac{1}{2}\sum_{n=3}^{\infty} \gamma^{n-1} \log n \approx 0.24985$$

and $\sigma^2 \approx 0.08007$. The number of connected spanning subgraphs is very similar, except that $w(B) = \log(|B|+1)$ for $|B| > 2$. We get an analogous result with $\mu \approx 0.29690$ and $\sigma^2 \approx 0.12113$.

A.2 Block graphs

Block graphs are similar to cacti: every block is a complete graph. Thus there is precisely one type of block for every size. Since there is only one way of labelling a complete graph, the block generating function is

$$B(z) = \sum_{n=2}^{\infty} \frac{1}{n!} z^n = e^z - z - 1.$$

Therefore, $\gamma \approx 0.56714$ is the positive real solution to the equation $ze^z = 1$, and $\rho \approx 0.26438$. We consider several block statistics again:

Number of blocks

Again, the formulas given in (10) apply, and we have $\mu \approx 0.76322$ and $\sigma^2 \approx 0.12512$ in Theorem 3.

Number of edges

For the number of edges, we now have to take $w(B) = \binom{|B|}{2}$. As a result, we obtain

$$\mu = B_{zt}(\gamma, 0) = \sum_{n=2}^{\infty} \binom{n}{2} \frac{1}{(n-1)!} \gamma^{n-1} = \Big(\gamma + \frac{\gamma^2}{2}\Big) e^{\gamma} = 1 + \frac{\gamma}{2} \approx 1.28357.$$

Similar calculations for higher order partial derivatives of B yield $\sigma^2 = \frac{\gamma(\gamma^2+2\gamma+2)}{4(\gamma+1)} \approx 0.31267$.

Number of spanning trees

For the (logarithm of the) number of spanning trees, we need to take $w(B) = (|B|-2)\log|B|$, since a complete graph with b vertices has b^{b-2} spanning trees. It follows that

$$\mu = B_{zt}(\gamma, 0) = \sum_{n=2}^{\infty} \frac{(n-2)\log n}{(n-1)!} \gamma^{n-1} \approx 0.28580,$$

and we find the numerical value of σ^2 to be 0.23671.

Number of complete subgraphs

The number of complete subgraphs is an example of a block statistic whose weight function has exponential growth. However, since the block generating function has radius of convergence $\eta = \infty$ in this case, the conditions of Theorem 3 are still clearly satisfied. We have $w(B) = 2^{|B|} - |B| - 1$ in this case: recall here that we are only counting nontrivial complete subgraphs with at least two vertices – if we want to count all complete subgraphs, we only need to add the number of vertices, which is a deterministic quantity in our setting.

It follows that Theorem 3 applies with

$$\mu = B_{zt}(\gamma, 0) = 2e^{2\gamma} - (\gamma+2)e^{\gamma} = \frac{2 - 2\gamma - \gamma^2}{\gamma^2} \approx 1.69146$$

and (by a similar calculation) $\sigma^2 = \frac{12\gamma^3 - 24\gamma^2 + 4\gamma + 4}{\gamma^4(\gamma+1)} \approx 4.55177$.

A.3 Series-parallel graphs

Series-parallel graphs are the most complicated example that we consider, since the block generating function can only be defined implicitly in terms of generating functions in two variables z and y, respectively marking the number of vertices and edges.

In fact, each block b with a distinguished vertex admits a tree-like decomposition $\tau(b)$ into components that are either of types *ring* or *multi-edge*, where the nodes of $\tau(b)$ correspond to the different components of b. We refer the reader to [2] for more details. Using then a vertex-distinguished version of the *dissymmetry theorem for tree-decomposable classes* (see [2, Section 5.3.3]), one can relate the generating function of blocks with a distinguished vertex to the generating functions $T^{(r)}(z,y)$, $T^{(m)}(z,y)$ and $T^{(rm)}(z,y)$ of their associated tree-decompositions, respectively rooted at a node of type ring, multi-edge or at an edge between a ring and a multi-edge node.

Those generating functions are in turn expressed in terms of $D(z,y)$, the generating function of series-parallel *networks*, i.e. 2-connected graphs with a pair of distinguished vertices called its *poles*. Such networks can either be the single edge, with generating function y, or of types *series*, with generating function $S(z,y)$, or *parallel*, with generating function $P(z,y)$, see [1] for a detailed exposition. Altogether, this gives:

$$\begin{aligned}
B_z(z,y) &= zy + T^{(r)}(z,y) + T^{(m)}(z,y) - T^{(rm)}(z,y),\\
T^{(r)}(z,y) &= zS(z,y)(D(z,y) - S(z,y))/2,\\
T^{(m)}(z,y) &= zP(z,y) - zyS(z,y) - zS^2(z,y)/2,\\
T^{(rm)}(z,y) &= zS(z,y)P(z,y),\\
D(z,y) &= y + S(z,y) + P(z,y),\\
S(z,y) &= zD(z,y)(D(z,y) - S(z,y)),\\
P(z,y) &= y\exp(S(z,y)) - y + \exp(S(z,y)) - S(z,y) - 1.
\end{aligned} \tag{11}$$

From the last three equations of (11) we obtain an implicit equation defining $D(z,y)$. Furthermore, one can write $B_z(z,y)$ in terms of $D(z,y)$ only. This gives:

$$\begin{aligned}
D(z,y) &= (1+y)e^{\frac{zD(z,y)^2}{1+zD(z,y)}} - 1,\\
B_z(z,y) &= \frac{zD(z,y)(2 - zD(z,y)^2)}{2zD(z,y)+2}.
\end{aligned} \tag{12}$$

So any partial derivative of $B_z(x,y)$ can be computed from the system (12). In particular, we get numerically that $\gamma \approx 0.12797$.

Number of blocks

For the number of blocks, one now sets $y = 1$ and $w(B) = 1$ in (12). The required conditions are satisfied, so we obtain a central limit theorem. In this case, the numerical values μ and σ^2 are 0.14937 and 0.14875 respectively.

Number of edges

Although the number of edges is now no longer just dependent on the number of vertices of a block, it is already controlled by the variable $y = e^t$ in the decomposition given in (12). We obtain a central limit theorem with $\mu \approx 1.61673$ and $\sigma^2 \approx 0.21125$ (cf. [1]).

Number of spanning trees

The number of spanning trees in series-parallel graphs was studied in a paper by Ehrenmüller and Rué [7]. They determined an asymptotic formula for the mean, but no limit distribution. As we find by means of our general result now, the distribution of the number of spanning trees in series-parallel graphs is asymptotically lognormal. Letting $\tau(G)$ be the number of spanning trees of a graph G, we simply set $w(B) = \log \tau(B)$ for all blocks (as for the other two graph classes), so that $S_w(G) = \log \tau(G)$. The conditions of Theorem 3 are clearly satisfied again, but the constants μ and σ^2 are rather difficult to evaluate in this example, as they can no longer be expressed directly by means of functional equations. Moreover, the infinite series

$$\mu = B_{zt}(\gamma, 0) = \sum_{B \in \mathcal{B}} \frac{w(B)\gamma^{|B|-1}}{(|B|-1)!}$$

converges poorly in this example, since $\gamma \approx 0.12797$ is only a little smaller than the radius of convergence of $B(z, 0)$, which is $\eta \approx 0.12800$. Therefore, the series representation is also not suitable to compute a numerical approximation, as determining $w(B) = \log \tau(B)$ for all blocks up to a certain size is rather costly.

On the Probability That a Random Digraph Is Acyclic

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Abstract

Given a positive integer n and a real number $p \in [0, 1]$, let $\mathcal{D}(n, p)$ denote the random digraph defined in the following way: each of the $\binom{n}{2}$ possible edges on the vertex set $\{1, 2, 3, \ldots, n\}$ is included with probability $2p$, where all edges are independent of each other. Thereafter, a direction is chosen independently for each edge, with probability $\frac{1}{2}$ for each possible direction. In this paper, we study the probability that a random instance of $\mathcal{D}(n, p)$ is *acyclic*, i.e., that it does not contain a directed cycle. We find precise asymptotic formulas for the probability of a random digraph being acyclic in the sparse regime, i.e., when $np = O(1)$. As an example, for each real number μ, we find an exact analytic expression for $\varphi(\mu) = \lim_{n\to\infty} n^{1/3}\mathbb{P}\left\{\mathcal{D}\left(n, \frac{1}{n}(1 + \mu n^{-1/3})\right) \text{ is acyclic}\right\}$.

2012 ACM Subject Classification Mathematics of computing → Random graphs; Mathematics of computing → Generating functions

Keywords and phrases Random digraphs, acyclic digraphs, asymptotics

Digital Object Identifier 10.4230/LIPIcs.AofA.2020.25

Funding *Dimbinaina Ralaivaosaona*: Supported by Division for Research Development (DRD) of Stellenbosch University and the National Research Foundation (NRF) of South Africa.
Stephan Wagner: Supported by the Knut and Alice Wallenberg Foundation.

Acknowledgements We want to thank the DSI-NRF Centre of Excellence in Mathematical and Statistical Sciences (CoE-MaSS), South Africa, for partially funding Vonjy Rasendrahasina's visit to Stellenbosch University in December 2018.

1 Introduction

By a *simple digraph*, we mean a digraph (directed graph) without loops, (directed) 2-cycles or multiple edges. Such a digraph is called *acyclic* if it has no directed cycles, i.e., cycles that follow the direction of the edges. One easily observes that the only strongly connected components of an acyclic digraph are its vertices. Acyclic digraphs form an important class of digraphs that occurs naturally in many applications, such as scheduling or Bayesian networks.

The enumeration of acyclic digraphs is a classical combinatorial problem that was first considered in the 1970s, see Harary and Palmer [17], Liskovec [23, 24], Robinson [31, 32] and Stanley [34]. It is based on a recursion for the number of acyclic digraphs, which we briefly recall here. Let a_n denote the number of acyclic digraphs on n (labelled) vertices.

Distinguishing by the number of sinks (vertices without an outgoing edge; equivalently, one can also consider sources, which are vertices without an incoming edge) and applying an elegant inclusion-exclusion argument, one finds that

$$a_n = \sum_{k=1}^{n} (-1)^{k-1} \binom{n}{k} 2^{k(n-k)} a_{n-k}$$

for $n > 1$, with initial value $a_0 = 1$. This can be rewritten as

$$\sum_{k=0}^{n} \frac{(-1)^k}{k!(n-k)!} 2^{-\binom{k}{2}-\binom{n-k}{2}} a_{n-k} = \begin{cases} 1 & n = 0, \\ 0 & n > 0. \end{cases}$$

Introducing the *special generating function* $A(x) = \sum_{n\geq 0} \frac{1}{n!} 2^{-\binom{n}{2}} a_n x^n$, one finds that

$$A(x) = \frac{1}{\sum_{n\geq 0} \frac{(-1)^n}{n!} 2^{-\binom{n}{2}} x^n}.$$

It can be shown that this function is meromorphic, and that the pole with minimum modulus occurs at $x \approx 1.48808$. From this, one can derive the asymptotic formula

$$\frac{a_n}{n!} 2^{-\binom{n}{2}} \sim C \cdot B^n,$$

where $C \approx 1.74106$ and $B \approx 0.67201$. These results can be found in the work of Robinson [31] (see also Liskovec [23] and Stanley [34]).

It is not difficult to include the number of edges in the count: let $a_{n,m}$ denote the number of labelled acyclic digraphs with n vertices and m edges, and set

$$A(x, y) = \sum_{n,m\geq 0} \frac{1}{n!} (1 + y)^{-\binom{n}{2}} a_{n,m} x^n y^m. \tag{1}$$

Then, we can also write this bivariate generating function in a reciprocal form:

$$A(x, y) = \frac{1}{\phi(x, y)}, \quad \text{where } \phi(x, y) = \sum_{k=0}^{\infty} \frac{(-x)^k}{k!\,(1 + y)^{\binom{k}{2}}}. \tag{2}$$

This was already observed by Robinson in [31]. Bender, Richmond, Robinson and Wormald [1] exploited this generating function identity to prove asymptotic formulas for the number of acyclic digraphs with a given number of vertices and edges if the number of edges is "large" (i.e., quadratic in the number of edges). In particular, it is shown in [1] that the number of edges in a random acyclic digraph with n vertices satisfies a central limit theorem with mean $\sim \frac{n^2}{4}$ and variance $\sim \frac{n^2}{8}$.

Next, let us discuss models of random digraphs. $\mathbb{D}(n, p)$ denotes a directed digraph on n labelled vertices in which each of the $n(n-1)$ directed edges is present with probability p, independently of the others, as described in [20, 26]. The model exhibits a phase transition that is somewhat similar to the *binomial model* $\mathbb{G}(n, p)$ of undirected graphs. This phase transition was, among others, studied by Karp [20] and Łuczak [25]. They proved the following: if np is fixed with $np < 1$ then every strong component has at most $\omega(n)$ vertices, for any sequence $\omega(n)$ tending to infinity arbitrarily slowly, and all strong components are either cycles or single vertices. If np is fixed with $np > 1$, then there exists a unique strong component of linear size, while all the other strong components are of logarithmic size (see also [15, Chapter 13]). Recently, Łuczak and Seierstad [26] obtained more precise results about the width and behaviour of the window where the phase transition occurs. They established that the scaling window is given by $np = 1 + \mu n^{-1/3}$, where μ is fixed. There, the largest strongly connected components have size of order $n^{1/3}$. Bounds on the tail probabilities of the distribution of the size of the largest component are also given by Coulson [7].

We use a slightly different model of random digraphs that has already been considered in similar contexts: first, we generate a random undirected graph according to the classical Erdős-Rényi model, where each of the possible $\binom{n}{2}$ edges between n fixed vertices is inserted with the same probability $2p$ and all edges are independent of each other. Thereafter, each edge is given a direction, where each of the two directions has probability $\frac{1}{2}$ and all choices are made independently again. Note that each possible directed edge is present in the graph with the same probability p in this model. The result is a random digraph without loops, multiple edges and 2-cycles (the latter is relevant since the presence of 2-cycles would immediately mean that the digraph is not acyclic). The random digraph generated in this way is denoted by $\mathcal{D}(n, p)$, and we ask the simple question: with what probability is $\mathcal{D}(n, p)$ acyclic? Throughout this paper, this probability will be denoted by $\mathbb{P}(n, p)$. In the case where p is of constant order, the asymptotic behaviour of $\mathbb{P}(n, p)$ can be inferred from the aforementioned results of Bender, Richmond, Robinson and Wormald. In this paper, however, we will be interested in the sparse regime, where $p = \lambda/n$ for some fixed real λ. In this case, the number of edges is only linear in n, resulting in a much higher probability of being acyclic. There is no particular reason why we chose to work with $\mathcal{D}(n, p)$ in this paper. Both models have appeared in the literature, but due to lack of space we only treat one model here. We will include $\mathbb{D}(n, p)$ in the long version of this paper.

Before we get to the statement of our main result, let us also review some related works. The model $\mathcal{D}(n, p)$ of simple random digraphs was used by Subramanian in [30], where the author studied induced acyclic subgraphs in random digraphs for fixed p. Following this work, there are also some relatively recent results on the related question of the largest acyclic subgraph in random digraphs in the stated range [9–11, 33].

The structure of the strong components of a random digraph for the $\mathbb{D}(n, p)$ model has been studied by many authors in the dense case, i.e., when $np \to \infty$ as $n \to \infty$. The largest strong components in a random digraph with a given degree sequence are studied by Cooper and Frieze [4] and the strong connectivity of an inhomogeneous random digraph was studied by Bloznelis, Göetze and Jaworski in [3]. The hamiltonicity of $\mathbb{D}(n, p)$ was investigated by Hefetz, Steger and Sudakov [18] and by Ferber, Nenadov, Noever, Peter and Škorić [13], by Cooper, Frieze and Molloy [5] and by Ferber, Kronenberg and Long [12]. Krivelevich, Lubetzky and Sudakov [21] also proved the existence of cycles of linear size with high probability (w.h.p.) when np is large enough.

Interestingly, since the enumeration of acyclic digraphs by Robinson [31] and the asymptotic results on acyclic digraphs by Bender et al. [1, 2], dense random graphs have been the focus of research in this context. However, a forthcoming independent approach of De Panafieu and Dovgal [8] gives a characterization of the probability that a digraph is acyclic inside the critical window using techniques from analytic combinatorics and the uniform model for digraphs.

Returning to the functional equation relating $A(x, y)$ and $\phi(x, y)$ in (2), it is clear that the behaviour of the zeros of $\phi(x, y)$ plays an important role in the study of acyclic digraphs. Here, by a zero of $\phi(x, y)$ we mean a function $x = x(y)$ that satisfies $\phi(x, y) = 0$. The properties of these zeros are certainly interesting in their own right. There are some known results in this direction. It is, for example, known that all zeros of ϕ are real, positive and distinct when $y > 0$, see [22, 29]. For a given $y > 0$ and $j \in \mathbb{N}$, let $\varrho_j(y)$ be the j-th smallest solution to the equation $\phi(x, y) = 0$. So, as mentioned before, we have $\varrho_1(1) \approx 1.48808$. Grabner and Steinsky [16] studied the behaviour of the other zeros of $\phi(x, 1)$, extending the work of Robinson. Our first result provides asymptotic formulas for the zeros of ϕ as $y \to 0^+$.

▶ **Theorem 1.** *Let $\phi(x, y)$ be the function defined in (2). For a given y, let $\varrho_j(y)$ be the solution to the equation $\phi(x, y) = 0$ that is the j-th closest to zero. If $j \in \mathbb{N}$ is fixed, then we have*

$$\varrho_j(y) = \frac{1}{e} y^{-1} - \frac{a_j}{2^{1/3} e}\, y^{-1/3} - \frac{1}{6e} + O(y^{1/3}), \quad \text{as } y \to 0^+, \tag{3}$$

where a_j is the zero of the Airy function $\mathrm{Ai}(z)$ that is j-th closest to 0. Furthermore, we have the following estimate for the partial derivative of $\phi(x, y)$ at $\varrho_j(y)$:

$$\phi_x(\varrho_j(y), y) \sim -\kappa_j\, y^{1/6} \exp\left(-\tfrac{1}{2} y^{-1} + 2^{-1/3} a_j\, y^{-1/3}\right) \ \text{as } y \to 0^+, \tag{4}$$

where

$$\kappa_j = \pi^{1/2} 2^{7/6} e^{11/12} \mathrm{Ai}'(a_j).$$

Using Theorem 1, we are able to obtain the following result on the probability that $\mathcal{D}(n, p)$ has no directed cycles.

▶ **Theorem 2.** *Let $p = \lambda/n$ with $\lambda \geq 0$ fixed. Then, the probability $\mathbb{P}(n, p)$ that a random digraph $\mathcal{D}(n, p)$ is acyclic satisfies the following asymptotic formulas as $n \to \infty$:*

$$\mathbb{P}(n, p) \sim \begin{cases} (1-\lambda) e^{\lambda + \lambda^2/2} & \text{if } 0 \leq \lambda < 1, \\ \gamma_1 n^{-1/3} & \text{if } \lambda = 1, \\ \gamma_2 n^{-1/3} e^{-c_1 n - c_2 n^{1/3}} & \text{if } \lambda > 1, \end{cases} \tag{5}$$

where

$$\gamma_1 = \frac{2^{-1/3} e^{3/2}}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\mathrm{Ai}(-i 2^{1/3} t)} \mathrm{d}t \approx 2.19037,$$

$$\gamma_2 = \tfrac{2^{-2/3}}{\mathrm{Ai}'(a_1)} \lambda^{5/6} e^{-\lambda^2/4 + 8\lambda/3 - 11/12},$$

$$c_1 = \tfrac{\lambda^2 - 1}{2\lambda} - \log \lambda,$$

$$c_2 = 2^{-1/3} a_1 \lambda^{-1/3} (1 - \lambda),$$

and a_1 is the zero of the Airy function $\mathrm{Ai}(z)$ with the smallest modulus.

We are also able to determine an asymptotic formula for the probability $\mathbb{P}(n, p)$ in the critical window, i.e., when $np = 1 + \mu n^{-1/3}$ and μ is bounded. This result is formulated in the next theorem.

▶ **Theorem 3.** *If $np = 1 + \mu n^{-1/3}$ such that μ is contained in a fixed bounded real interval, then*

$$\mathbb{P}(n, p) = (\varphi(\mu) + o(1)) n^{-1/3}, \quad \text{as } n \to \infty, \tag{6}$$

where

$$\varphi(\mu) = 2^{-1/3} e^{3/2 - \mu^3/6} \times \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \frac{e^{-\mu s}}{\mathrm{Ai}(-2^{1/3} s)} \mathrm{d}s. \tag{7}$$

The term that follows after "×" in Equation (7) is an inverse (two-sided) Laplace transform. Hence, the function $2^{1/3}e^{\mu^3/6-3/2}\varphi(\mu)$ can be interpreted as the inverse (two-sided) Laplace transform of the function $\mathrm{Ai}(-2^{1/3}s)^{-1}$. We provide a numerical plot of $\varphi(\mu)$ in Figure 1.

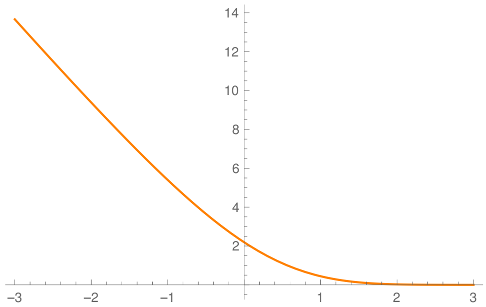

Figure 1 Numerical plot of $\varphi(\mu)$.

Throughout this paper, we use the Vinogradov notation $\ll$ interchangeably with the O-notation, i.e., as $x \to a$ (resp. $x \to \infty$), $f(x) \ll g(x)$ and $f(x) = O(g(x))$ both mean that there exists $C > 0$ independent of x such that $|f(x)| \le Cg(x)$ for all x sufficiently close to a (resp. all sufficiently large $x > 0$).

2 Estimates of $\phi(x, y)$ and its zeros

The main ingredients in the proofs of our theorems are asymptotic estimates for $\phi(x, y)$ as $y \to 0^+$, for various ranges of x, including complex values. These estimates are given in Proposition 4 and Proposition 7. The proofs of these propositions are long and rather technical, so we will not include them in this extended abstract. However, sketched proofs are provided in the Appendix. The proofs are based on the saddle-point method as it is possible to express $\phi(x, y)$ in an integral form via a formula due to Mahler [27].

2.1 Mahler's transformation

The function $\phi(x, y)$ can be expressed in terms of the function $F(z)$ in [27, Equation (6)]. In fact, they are equal if we set $z = -x$ and $q = (1 + y)^{-1}$. Thus using the integral form of $F(z)$ in [27, Equation (4)] we obtain the following formula:

$$\phi(x,y) = \sqrt{\frac{\log(1+y)}{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\log(1+y)z^2 - x(1+y)^{1/2-iz}\right) \mathrm{d}z. \tag{8}$$

It is worth noting that this equation can also derived from [14, Lemma 1]. To simplify this expression, from now on, we shall use the abbreviations

$$\alpha := \log(1+y) \quad \text{and} \quad \beta := \sqrt{1+y}. \tag{9}$$

Moreover, by making the change of variable $z \mapsto z/\alpha$, we can rewrite Equation (8) as

$$\phi(x,y) = \frac{1}{\sqrt{2\pi\alpha}} \int_{-\infty}^{\infty} e^{f(z)}\mathrm{d}z, \quad \text{where } f(z) := -\frac{1}{2\alpha}z^2 - x\beta e^{-iz}. \tag{10}$$

The function f depends on the variables x and y, but we drop these dependencies in the notation for easy reading. In addition, when we say derivative of f, we always mean derivative with respect to z. In the rest of this section, we assume that x is real.

2.2 Saddle-point method

The integral in the formula for $\phi(x, y)$ in (10) is an integral over the real line. However, since the function f is entire as a function of z, we can change this path of integration without affecting the validity of the equation (Figure 2 in the appendix shows the paths that we considered). This allows us to apply the saddle-point method to the integral (10). The objective is to find a path that goes through a saddle-point, i.e., a solution of $f'(z) = 0$. Since the derivative of f is $f'(z) = -\frac{1}{\alpha}z + ix\beta e^{-iz}$, we can see that $f'(z) = 0$ if and only if

$$ize^{iz} = -x\alpha\beta. \tag{11}$$

Hence, the solutions can be expressed in terms of the branches of the Lambert-W function, which is implicitly defined by the equation $\mathrm{W}(s)e^{\mathrm{W}(s)} = s$. We choose a solution to Equation (11) that is given by the principal branch of W. So, set

$$w := W_0(-x\alpha\beta) \ \text{ and } z_0 := -iw, \tag{12}$$

where W_0 is the principal branch of the Lambert function. Note that z_0 still depends on the variables x and y. The fact that the Lambert function $W_0(z)$ has a singularity at $z = -1/e$ suggests that we should consider x to be a function of y such that $x\alpha\beta$ is close to $1/e$. Motivated by this, let us define x_0 and δ such that

$$x_0 = \frac{1}{e\alpha\beta} \ \text{ and } \ x = (1+\delta)x_0. \tag{13}$$

With this setting, we are now able to give asymptotic estimates of $\phi(x, y)$ when $y \to 0^+$ for several ranges of δ. This result is summarized in the following proposition.

▶ **Proposition 4.** *If x is of the form $x = (1+\delta)x_0$, then $\phi(x, y)$ satisfies the following asymptotic formulas as $y \to 0^+$:*

(a) *If $\delta \geq -1$ and $\delta = -1 + o(1)$, then*

$$\phi(x, y) \sim e^{\frac{1}{2\alpha}(w^2+2w)}. \tag{14}$$

(b) *If $\delta < 0$ and $\alpha^{2/3} \ll |\delta| \leq 1 - \varepsilon$ for some constant $\varepsilon > 0$, then*

$$\phi(x, y) \sim 2^{5/6}\pi^{1/2}\alpha^{-1/6}|w|^{-1/3}\mathrm{Ai}(R)e^{\frac{2}{3}R^{3/2}+\frac{1}{2\alpha}(w^2+2w)} \tag{15}$$

where

$$R = 2^{-2/3}(1+w)^2 w^{-4/3}\alpha^{-2/3}.$$

(c) *If we let $\delta = \theta\alpha^{2/3}$, then*

$$\phi(x, y) = 2^{-1/2}\pi^{-1/2}\alpha^{-1/6}\left(K_1(\theta) + K_2(\theta)\,\alpha^{1/3} + O(\alpha^{2/3})\right) e^{-\frac{1}{2}\alpha^{-1}-\theta\alpha^{-1/3}}, \tag{16}$$

uniformly for θ in any fixed bounded closed interval, where

$$K_1(\theta) = \pi 2^{4/3}\mathrm{Ai}(-2^{1/3}\theta),$$
$$K_2(\theta) = \tfrac{5}{3}\pi\, 2^{1/3}\theta^2\mathrm{Ai}(-2^{1/3}\theta) - \tfrac{1}{3}\pi 2^{2/3}\mathrm{Ai}'(-2^{1/3}\theta).$$

Proof. A sketch of the proof is given in the appendix. ◀

Observe that there is an overlap in the conditions of Part (b) and Part (c), but one can show that the asymptotic formulas (15) and (16) agree in the overlap. To check this, one needs to use the classic asymptotic formula for the Airy function $\mathrm{Ai}(z)$ as well as the asymptotic formula for $W_0(z)$ near its singularity $-1/e$. These are well known facts, see for example [28, (9.7.5)] and [6, (4.22)]. Since these estimates will be referred to quite often in this paper, let us state them here. For any $\varepsilon > 0$,

$$\mathrm{Ai}(z) \sim \frac{e^{-\frac{2}{3}z^{3/2}}}{2\sqrt{\pi}z^{1/4}} \quad \text{as } |z| \to \infty, \text{ and } |\mathrm{Arg}(z)| \leq \pi - \varepsilon. \tag{17}$$

As for the Lambert function, as $z \to -1/e$, we have

$$W_0(z) = -1 + p - \frac{1}{3}p^2 + \frac{11}{72}p^3 + \cdots \tag{18}$$

where $p = \sqrt{2(ez+1)}$ (here, $\sqrt{\cdot}$ denotes the principal branch of the square root function).

We are now ready to prove Theorem 1.

2.3 Proof of Theorem 1

Proof. We already know that the zeros of $\phi(x, y)$ are real and positive. Observe that the main terms of $\phi(x, y)$ in Part (a) and Part (b) of Proposition 4 cannot vanish (in Part (b), R is always positive, which implies $\mathrm{Ai}(R) \neq 0$). However for Part (c), the term $K_1(\theta)$ in (16) can be zero, and this happens precisely when $\theta = -2^{-1/3}a_j$, where a_j is one of the zeros of $\mathrm{Ai}(z)$.

If we let $x = (1 + \theta\alpha^{2/3})x_0$, and make θ vary in a small interval around $-2^{-1/3}a_j$, then the main term of $\phi(x, y)$ changes sign. So by the intermediate value theorem there must be a zero close to $(1 - 2^{-1/3}a_j\alpha^{2/3})x_0$. The asymptotic formula of such a zero can be obtained by a simple bootstrapping argument using (16). This eventually gives an asymptotic formula of the form

$$\frac{1}{e}y^{-1} - \frac{a_j}{2^{1/3}e}y^{-1/3} - \frac{1}{6e} + O(y^{1/3}), \quad \text{as } y \to 0^+. \tag{19}$$

To show that there is only one zero that satisfies this asymptotic formula for every a_j, we make use of the functional equation

$$\phi_x(x, y) = -\phi\left((1 + y)^{-1}x, y\right),$$

which follows easily from the definition of $\phi(x, y)$ in (2). Now, suppose that there are two different zeros ϱ' and ϱ'' that both satisfy (19) for the same j. Then by Rolle's theorem, there exists C between ϱ' and ϱ'' (which also means that C satisfies the asymptotic formula (19)) such that $(1 + y)^{-1}C$ is a zero of ϕ. This leads to a contradiction, because if C satisfies (19) then $(1+y)^{-1}C$ does not (not even if a_j is replaced by another zero of the Airy function) if y is sufficiently small. So $(1 + y)^{-1}C$ cannot be a zero of $\phi(x, y)$.

Now that we have established that there is only one zero of $\phi(x, y)$ that satisfies (19) for each fixed $j \in \mathbb{N}$ and sufficiently small y, we name it $\varrho_j(y)$. Finally, to estimate $\phi_x(\varrho_j(y), y)$ as $y \to 0^+$, we make use of the above functional equation again, which gives us

$$\phi_x(\varrho_j(y), y) = -\phi\left((1 + y)^{-1}\varrho_j(y), y\right).$$

Then, we use (19) and (16) to estimate the right-hand side. ◀

3 Proving Theorem 2 and Theorem 3

3.1 Case $0 \leq \lambda < 1$

▶ **Lemma 5.** *Consider the random digraph $\mathcal{D}(n,p)$ with $p = \lambda/n$ and $0 \leq \lambda < 1$ fixed. Let X_n be the total number of (directed) cycles in this graph. Then,*
(a) *w.h.p., all strong components of $\mathcal{D}(n,p)$ are either cycles or single vertices.*
(b) *the number of vertices on a cycle is at most ω, for any $\omega(n) \to \infty$.*
(c) *X_n converges in distribution to $\mathrm{Po}(-\log(1-\lambda) - \lambda - \frac{\lambda^2}{2})$.*

Proof. If there is a strong component that is not a cycle or a single vertex, then there are three internally disjoint paths connecting two vertices u and v such that two of them do not have the same orientation or there are two directed cycles with a common vertex. The expected number of such components is bounded above by

$$2\binom{n}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\binom{n}{i}i!p^{i+1}\binom{n}{j}j!p^{j+1}\binom{n}{k}k!p^{k+1} + \binom{n}{1}\sum_{i=2}^{n}\sum_{j=2}^{n}\binom{n}{i}i!p^{i+1}\binom{n}{j}j!p^{j+1}$$
$$\leq \frac{\lambda^3}{n}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\lambda^{i+j+k} + \frac{\lambda^2}{n}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\lambda^{i+j} = O(n^{-1}).$$

By the Markov inequality, this means that there are, w.h.p., no such components.

For (b), we can bound the expected number of cycles of length larger than ω by

$$\sum_{k=\omega}^{n}\binom{n}{k}(k-1)!p^k = \sum_{k=\omega}^{n}\frac{\prod_{i=0}^{k-1}(n-i)}{n^k}\frac{\lambda^k}{k} \leq \sum_{k=\omega}^{n}\lambda^k = O\left(\lambda^{\omega}\right).$$

As $0 < \lambda < 1$, (b) follows from the Markov inequality.

Now to tackle (c), we compute first the expectation of X_n. Here, we have

$$\mathbb{E}\left[X_n\right] = \sum_{k=3}^{n}\binom{n}{k}(k-1)!p^k.$$

It follows that

$$\lim_{n\to\infty}\mathbb{E}(X_n) = \lim_{n\to\infty}\sum_{k=3}^{n}\frac{\prod_{i=0}^{k-1}(n-i)}{n^k}\frac{\lambda^k}{k} \sim \sum_{k=3}^{\infty}\frac{\lambda^k}{k} = -\log(1-\lambda) - \lambda - \frac{\lambda^2}{2} = a(\lambda).$$

Since the falling factorial $(X_n)_r = X_n(X_n-1)\cdots(X_n-r+1)$ counts the number of ordered r-tuples of r disjoint cycles, the r-th factorial moment of X_n is

$$\mathbb{E}\left[(X_n)_r\right] = \sum_{k_1=3}^{n}\sum_{k_2=3}^{n-k_1}\cdots\sum_{k_r=3}^{n-\sum_{i=1}^{r-1}k_i}\binom{n}{k_1,k_2,\ldots,k_r,n-k_1-\cdots-k_r}\prod_{i=1}^{r}(k_i-1)!p^{k_i}.$$

Without going into the technical details, one can now use the statement in (b) to show that the summations can be taken to ∞. One finds that for fixed $r \geq 2$, the r-th factorial moment $\mathbb{E}\left[(X_n)_r\right]$ is asymptotically equivalent to $a(\lambda)^r$ as $n \to \infty$. So by means of [19, Corollary 6.8], we have convergence to a Poisson distribution of parameter $a(\lambda)$. ◀

Now, the case $0 \leq \lambda < 1$ of Theorem 2 is a simple consequence of Lemma 5. Indeed Part (c) of Lemma 5 implies that

$$\lim_{n\to\infty}\mathbb{P}(n,p) = \lim_{n\to\infty}\mathbb{P}\left(X_n = 0\right) = e^{-a(\lambda)} = (1-\lambda)e^{\lambda+\lambda^2/2}.$$

3.2 Case $\lambda \geq 1$

3.2.1 Preliminaries

Let us begin with a crucial lemma which relates the probability $\mathbb{P}(n,p)$ to the coefficient $[x^n]A(x,y)$.

▶ **Lemma 6.** *The probability $\mathbb{P}(n,p)$ that a random digraph $\mathcal{D}(n,p)$ is acyclic is given by*

$$\mathbb{P}(n,p) = n!(1-p)^{\binom{n}{2}}[x^n]A\left(x, \tfrac{p}{1-2p}\right). \tag{20}$$

Proof. Define $A_n(y) = \sum_{m=0}^{\binom{n}{2}} a_{n,m}y^m$ where $a_{n,m}$ is the number of acyclic digraphs with n vertices and m edges defined in (1). Therefore, we have

$$A(x,y) = \sum_{n\geq 0} A_n(y)(1+y)^{-\binom{n}{2}}\frac{x^n}{n!} \quad \text{and} \quad A_n(y) = n!(1+y)^{\binom{n}{2}}[x^n]A(x,y). \tag{21}$$

Since $\mathbb{P}(n,p)$ is defined to be the probability that $\mathcal{D}(n,p)$ is acyclic, we can express it as $\mathbb{P}(n,p) = \sum_D \mathbb{P}(\mathcal{D}(n,p) = D)$, where the sum runs over all acyclic digraphs on n fixed vertices. The probability $\mathbb{P}(\mathcal{D}(n,p) = D)$ does not depend on the structure of D but only on its number of edges. Hence, by distinguishing the number of edges, we have

$$\begin{aligned}\mathbb{P}(n,p) &= \sum_{m=0}^{\binom{n}{2}} a_{n,m}p^m(1-2p)^{\binom{n}{2}-m}\\ &= (1-2p)^{\binom{n}{2}}\sum_{m=0}^{\binom{n}{2}} a_{n,m}\left(\frac{p}{1-2p}\right)^m\\ &= (1-2p)^{\binom{n}{2}}A_n\left(\frac{p}{1-2p}\right).\end{aligned}$$

Applying (21) with y replaced by $p/(1-2p)$, we get after a bit of algebra that the last term is the same as the right-hand side of Equation (20). ◀

By Lemma 6, it suffices to estimate the coefficient $[x^n]A(x,y)$ when y is of order n^{-1}. To this end, we use the Cauchy integral formula

$$[x^n]A(x,y) = \frac{1}{2\pi i}\oint_{|x|=\rho}\frac{A(x,y)}{x^{n+1}}\mathrm{d}x = \frac{1}{2\pi i}\oint_{|x|=\rho}\frac{1}{\phi(x,y)x^{n+1}}\mathrm{d}x, \tag{22}$$

where $0 < \rho < \varrho_1(y)$. Notice that x here is a complex variable, so in order to estimate $[x^n]A(x,y)$ via the above integral, we need an estimate of $\phi(x,y)$ where x is complex and $y \to 0^+$. This is done in the next proposition.

▶ **Proposition 7.** *Let θ be a fixed real number which satisfies $\mathrm{Ai}(-2^{1/3}\theta) \neq 0$ and let $\delta = \theta\alpha^{2/3}$. Moreover, let*

$$x = (1+\delta)x_0e^{iu}, \ \text{and } w = W_0(-(1+\delta)e^{iu-1}).$$

Then, we have the following asymptotic formulas for $\phi(x,y)$ as $y \to 0^+$:

(a) *If $\alpha^{1/2} \ll |u| \leq \pi$, then*

$$\phi(x,y) \sim \frac{e^{\frac{1}{2\alpha}(w^2+2w)}}{\sqrt{1+w}}. \tag{23}$$

(b) *If* $u = t\alpha^{2/3}$ *and* $1 \ll |t| \ll \alpha^{-1/6}$, *then*

$$\phi(x,y) \sim \pi^{1/2}\ 2^{5/6}\alpha^{-1/6}\mathrm{Ai}(-2^{1/3}(\theta+it))e^{-\frac{1}{2}\alpha^{-1}-(\theta+it)\alpha^{-1/3}-\frac{5}{6}\alpha^{1/3}t^2}. \tag{24}$$

(c) *If* $u = t\alpha^{2/3}$, *then the estimate*

$$\phi(x,y) \sim \pi^{1/2}\ 2^{5/6}\alpha^{-1/6}\mathrm{Ai}(-2^{1/3}(\theta+it))e^{-\frac{1}{2}\alpha^{-1}-(\theta+it)\alpha^{-1/3}} \tag{25}$$

holds uniformly for t *in any bounded closed interval on* $\mathbb{R}$.

Proof. A sketch of the proof is given in the appendix. ◀

▶ Remark 8. Once again, one can verify that these asymptotic formulas agree in those regions where conditions overlap.

The next lemma is a direct consequence of Proposition 7, which will be useful to estimate the integral in (22).

▶ **Lemma 9.** *Let* θ *be a fixed real number such that* $\mathrm{Ai}(-2^{1/3}\theta) \neq 0$, *and let* $\rho = (1+\theta\alpha^{2/3})x_0$. *Then, as* $y \to 0^+$,

$$\frac{1}{2\pi i}\oint_{|x|=\rho}\frac{1}{\phi(x,y)x^{n+1}}\mathrm{d}x \ll \frac{\alpha^{2/3}|\mathrm{Ai}(-2^{1/3}\theta)|}{2\pi\phi(\rho,y)\rho^n}\int_{-\infty}^{\infty}\frac{1}{|\mathrm{Ai}(-2^{1/3}(\theta+it))|}\mathrm{d}t, \tag{26}$$

where the implied constant is independent of n. *If we assume further that* n *and* α *are connected by a relation of the form* $n = \alpha^{-1} + b\alpha^{-2/3}$, *where* b *can be a function of* α *but with* $b = O(1)$, *then we have*

$$\frac{1}{2\pi i}\oint_{|x|=\rho}\frac{1}{\phi(x,y)x^{n+1}}\mathrm{d}x = \frac{\alpha^{2/3}\mathrm{Ai}(-2^{1/3}\theta)}{2\pi\phi(\rho,y)\rho^n}\left(\int_{-\infty}^{\infty}\frac{e^{-ibt}}{\mathrm{Ai}(-2^{1/3}(\theta+it))}\mathrm{d}t + o(1)\right). \tag{27}$$

Proof. We will only present the proof of the second estimate, which is the harder one, the idea of the proof of the first estimate will be very similar but simpler since it is only an upper bound. First, we have

$$\frac{1}{2\pi i}\oint_{|x|=\rho}\frac{1}{\phi(x,y)x^{n+1}}\mathrm{d}x = \frac{1}{2\pi\phi(\rho,y)\rho^n}\int_{-\pi}^{\pi}\frac{\phi(\rho,y)e^{-iun}}{\phi(\rho e^{iu},y)}\mathrm{d}u.$$

Next, we choose a fixed constant $c \in (1/2, 2/3)$, and we split the integral on the right-hand side into three pieces corresponding to each of the following ranges of u: $|u| \le \alpha^c$, $\alpha^c < |u| \le \alpha^{1/2}$, and $\alpha^{1/2} < |u| \le \pi$. Let us now treat these cases separately.

- If $\alpha^{1/2} < |u| \le \pi$, then we can use Part (a) of Proposition 7 to estimate $|\phi(\rho e^{iu},y)|$ and Part (c) of Proposition 4 to estimate $|\phi(\rho,y)|$. We get

  $$\left|\frac{\phi(\rho,y)e^{-iun}}{\phi(\rho e^{iu},y)}\right| \ll \alpha^{-1/6}\sqrt{|1+w|}\ e^{-\frac{1}{2}\alpha^{-1}\mathrm{Re}((1+w)^2)-\theta\alpha^{-1/3}},$$

  with w as defined in (12). Note that w is bounded in this case. Moreover, one can show (see Lemma 10 in the appendix) that $\mathrm{Re}((1+w)^2)$ remains positive if u is bounded away from zero, and by means of (18) (with $p = \sqrt{2(1-(1+\theta\alpha^{2/3})e^{iu})}$), one gets

  $$\mathrm{Re}((1+w)^2) = -2\theta\alpha^{2/3} + (1+o(1))\frac{4}{3}|u|^{3/2}, \tag{28}$$

  if $u \to 0$ and $|u| \ge \alpha^{1/2}$. Hence, we have

  $$-\frac{1}{2}\alpha^{-1}\mathrm{Re}((1+w)^2) - \theta\alpha^{-1/3} = -(\tfrac{2}{3}+o(1))\alpha^{-1}|u|^{3/2} \gg \alpha^{-1/4}$$

  uniformly for $\alpha^{1/2} < |u| \le \pi$. This implies that the contribution from $\alpha^{1/2} < |u| \le \pi$ to the above integral tends to zero exponentially quickly.

- If $\alpha^c < |u| \le \alpha^{1/2}$, then we use Part (b) of Proposition 7 to estimate $|\phi(\rho e^{iu}, y)|$. We obtain
$$\left|\frac{\phi(\rho, y)e^{-iun}}{\phi(\rho e^{iu}, y)}\right| \sim \frac{e^{\frac{5}{6}\alpha^{1/3}t^2}}{|\mathrm{Ai}(-2^{1/3}(\theta + it))|},$$
where $t = u\alpha^{-2/3}$. So, in particular $|t| > \alpha^{c-2/3}$. But since we chose $c < 2/3$, we have $|t| \to \infty$. Since θ is fixed, we have $|\mathrm{Arg}(-2^{1/3}(\theta + it))| \to \pi/2$. Therefore, by the asymptotic formula (17) for the Airy function, the contribution from $\alpha^c < |u| \le \alpha^{1/2}$ to the integral above is also tending to zero exponentially fast in α.
- If $|u| \le \alpha^c$, then we let $u = t\alpha^{2/3}$. So $\alpha^{1/3}t^2 = O(\alpha^{2c-1})$, which tends to zero. Also by the assumption on n in the statement of the lemma, we have
$$-iun = -it\alpha^{-1/3} - ibt.$$
Using Part (c) of Proposition 7 and $n = \alpha^{-1} + b\alpha^{-2/3}$, we get
$$\frac{\phi(\rho, y)e^{-iun}}{\phi(\rho e^{iu}, y)} \sim \frac{\mathrm{Ai}(-2^{1/3}\theta)e^{-ibt}}{\mathrm{Ai}(-2^{1/3}(\theta + it))}.$$
By making the change of variable $u = t\alpha^{2/3}$, we obtain
$$\int_{-\alpha^c}^{\alpha^c} \frac{\phi(\rho, y)e^{-iun}}{\phi(\rho e^{iu}, y)}\mathrm{d}u \sim \alpha^{2/3}\mathrm{Ai}(-2^{1/3}\theta)\int_{-\alpha^{c-2/3}}^{\alpha^{c-2/3}} \frac{e^{-ibt}}{\mathrm{Ai}(-2^{1/3}(\theta + it))}\mathrm{d}t.$$
Once again, by the asymptotic formula (17) for the Airy function, the integral on the right-hand side can be extended to infinity with an exponentially small error term, uniformly in b.

The proof of the asymptotic formula (27) is complete. ◀

We now have everything we need to complete the proof of Theorem 2 and to prove Theorem 3. Since the case $\lambda = 1$ in Theorem 2 is a particular case of Theorem 3, it does not need to be treated separately. Let us begin with a proof of Theorem 3.

3.2.2 Case $\lambda = 1 + \mu n^{-1/3}$

Let $np = 1 + \mu n^{-1/3}$, where μ is contained in a fixed bounded interval. In view of Lemma 6 we set $y = p/(1-2p)$, and with $\alpha = \log(1+y)$, we can show that n satisfies
$$n = \alpha^{-1} + \mu\alpha^{-2/3} + O(\alpha^{-1/3}).$$
We choose $\rho = x_0 = \frac{1}{e\alpha\beta}$ (which is smaller than $\varrho_1(y)$). Hence, by Equation (27) of Lemma 9 (with $\theta = 0$), we have
$$[x^n]A(x, y) = \frac{\alpha^{2/3}\mathrm{Ai}(0)}{2\pi\phi(\rho, y)\rho^n}\left(\int_{-\infty}^{\infty} \frac{e^{-i\mu t}}{\mathrm{Ai}(-2^{1/3}it)}\mathrm{d}t + o(1)\right).$$
Thus Lemma 6 yields
$$\mathbb{P}(n, p) = n!(1-p)^{\binom{n}{2}}\frac{\alpha^{2/3}\mathrm{Ai}(0)}{2\pi\phi(\rho, y)\rho^n}\left(\int_{-\infty}^{\infty} \frac{e^{-i\mu t}}{\mathrm{Ai}(-2^{1/3}it)}\mathrm{d}t + o(1)\right).$$
We apply Part (c) of Proposition 4 (or Part (c) of Proposition 7) to estimate $\phi(\rho, y)$, then write everything in terms of n. With the help of a computer algebra system (we used asymptotic expansions in SageMath [35]) we obtain the asymptotic formula
$$\mathbb{P}(n, p) = 2^{-1/3}e^{3/2-\mu^3/6}\,n^{-1/3} \times \frac{1}{2\pi}\left(\int_{-\infty}^{\infty} \frac{e^{-i\mu t}}{\mathrm{Ai}(-2^{1/3}it)}\mathrm{d}t + o(1)\right)$$
as $n \to \infty$, which is equivalent to the estimate of $\mathbb{P}(n, p)$ in Theorem 3.

3.2.3 Case $\lambda > 1$

Let $\lambda > 1$ be a fixed real number, and let $np = \lambda$. We follow the same argument as above, but we choose $\rho = (1 + \theta\alpha^{2/3})x_0$, where θ is fixed and satisfies $-a_1 < 2^{1/3}\theta < -a_2$. This implies that $\mathrm{Ai}(-2^{1/3}\theta) \neq 0$ and that $\varrho_1(y) < \rho < \varrho_2(y)$. Hence, by the residue theorem, we have

$$[x^n]A(x,y) = -\frac{1}{\varrho_1(y)^{n+1}\phi_x(\varrho_1(y),y)} + \frac{1}{2\pi i}\oint_{|x|=\rho} \frac{1}{\phi(x,y)x^{n+1}}\mathrm{d}x. \tag{29}$$

Then, we use (26) of Lemma 9 to estimate the integral on the right-hand side, so we get

$$[x^n]A(x,y) = -\frac{1}{\varrho_1(y)^{n+1}\phi_x(\varrho_1(y),y)} + O\left(\frac{\alpha^{2/3}}{|\phi(\rho,y)|\rho^n}\right).$$

In view of the formula $\mathbb{P}(n,p) = n!(1-p)^{\binom{n}{2}}[x^n]A(x,y)$, we can express the contribution to $\mathbb{P}(n,p)$ from each of the terms above in terms of n: we use Theorem 1 to estimate $\varrho_1(y)$ and $\phi_x(\varrho_1(y),y)$ and Part (c) of Proposition 4 to estimate $\phi(\rho,y)$. Then, with the help of a computer algebra system, we obtain

$$-\frac{n!(1-p)^{\binom{n}{2}}}{\varrho_1(y)^{n+1}\phi_x(\varrho_1(y),y)} \sim \gamma_2 n^{-1/3} e^{-c_1 n + 2^{1/3}a_1\lambda^{-1/3}(\lambda-1)n^{1/3}}, \tag{30}$$

$$\frac{n!(1-p)^{\binom{n}{2}}\alpha^{2/3}}{|\phi(\rho,y)|\rho^n} \ll n^{-1/3} e^{-c_1 n - \theta\lambda^{-1/3}(\lambda-1)n^{1/3}}, \tag{31}$$

where the constants γ_2 and c_1 are precisely as defined in Theorem 2. Since we chose θ in such a way that $\theta > -2^{-1/3}a_1$, the left-hand side of (31) is exponentially (in $n^{1/3}$) smaller than that of (30) as $n \to \infty$. Therefore, the right-hand side of (30) is indeed the main term of $\mathbb{P}(n,p)$.

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A Sketched Proof of Proposition 4

The proof is based on the saddle-point method applied to the integral in the formula for $\phi(x,y)$ in (10). Recall that we set $x = (1+\delta)x_0$, where $x_0 = (e\alpha\beta)^{-1}$. Note that the case $\delta = -1$ corresponds to $x = 0$, and so it immediately follows from the definition of $\phi(x,y)$ in (2) that $\phi(0,y) = 1$. Hence, we may assume that $\delta > -1$, but it can be a function of α. Recall the saddle-point z_0 defined in (12), $z_0 = -iw$, where $w = \mathrm{W}_0(-(1+\delta)e^{-1})$. One can see that if δ goes from -1 to 0, then w goes from 0 to -1. So if $\delta \in (-1, 0]$, then the point z_0 lies on the segment $[0,\ i]$. The Taylor series around z_0 is

$$f(z) = f(z_0) + f'(z_0)(z-z_0) + f''(z_0)\frac{(z-z_0)^2}{2!} + f'''(z_0)\frac{(z-z_0)^3}{3!} + \cdots$$

where

$$f(z_0) = -\frac{1}{2\alpha}z_0^2 + \frac{iz_0}{\alpha} = \frac{1}{2\alpha}(w^2+2w) \tag{32}$$

$$f''(z_0) = -\frac{1}{\alpha}(1+iz_0) = -\frac{1}{\alpha}(1+w) \tag{33}$$

$$f'''(z_0) = -\frac{z_0}{\alpha} = \frac{i}{\alpha}w \tag{34}$$

$$|f^{(k)}(\eta+z_0)| = \frac{|w|}{\alpha} \le \frac{1}{\alpha} \text{ for every } \eta \in \mathbb{R} \text{ and } k \ge 4. \tag{35}$$

Looking at the first few terms in the Taylor series above, note that the quadratic term $f''(z_0)(z-z_0)^2$ also vanishes when $z_0 = i$. So we proceed as follows: if z_0 is sufficiently far from i (for our case it means $|z_0 - i| \gg \alpha^{2/3}$), then we shift the path of integration to the horizontal line passing through z_0, and if $|z_0 - i| \ll \alpha^{2/3}$, then we take the path Γ on the right in Figure 2.

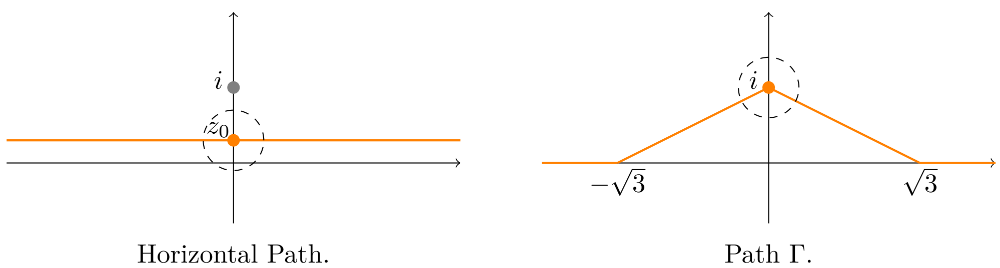

Figure 2 Two Paths.

We can use the path Γ in the integral (10) since $f(z)$ is an entire function. But we can also shift the path of integration to any horizontal line. To see this, for any real numbers a, b, (assuming that x is real for now) we have

$$\mathrm{Re}(f(a+ib)) = -\frac{1}{2\alpha}(a^2-b^2) - x\beta e^b\cos(a).$$

This implies that $|e^{f(z)}| = e^{\mathrm{Re}(f(z))}$ tends to zero exponentially fast as $|\mathrm{Re}(z)| \to \infty$ on any fixed horizontal strip for $\alpha > 0$. Hence we can shift the path of integration within this strip.

Before we begin proving each part of Proposition 4, let us adopt some terminology. The dashed circles in the two graphs in Figure 2 represent circles of radius α^c, where c is a positive constant. But c will be chosen separately for each range of x. The part of the integral from the path within the circle will be called the *local integral* and the rest will be called the *tail*.

A.1 Part (a)

Here, we assume that $\delta > -1$, but that the asymptotic formula $\delta = -1 + o(1)$ is satisfied as $\alpha \to 0^+$. Then, we choose $c \in (1/3, 1/2)$. To estimate the local integral, we have

$$f(t+z_0) = f(z_0) + f''(z_0)\frac{t^2}{2} + O(\alpha^{3c-1}),$$

for $|t| \le \alpha^c$, where the implicit constant in the O term is independent of t. This implies that

$$\int_{-\alpha^c}^{\alpha^c} e^{f(t+z_0)}\mathrm{d}t = (1 + O(\alpha^{3c-1}))e^{f(z_0)} \int_{-\alpha^c}^{\alpha^c} e^{f''(z_0)t^2/2}\mathrm{d}t.$$

The condition $\delta = -1 + o(1)$ implies that $w = o(1)$, hence $f''(z_0) \sim -\alpha^{-1}$. This allows us to extend the range of integration in the integral above to infinity at the expense of an exponentially small error term. Thus, we have

$$\int_{-\alpha^c}^{\alpha^c} e^{f(t+z_0)}\mathrm{d}t \sim e^{f(z_0)} \int_{-\infty}^{\infty} e^{f''(z_0)t^2/2}\mathrm{d}t \sim \sqrt{\frac{2\pi}{-f''(z_0)}}e^{f(z_0)}.$$

Now for the estimate of the tail. From the definition of the function $f(z)$, we can show that

$$\mathrm{Re}(f(t+z_0)) - f(z_0) = -\frac{1}{2\alpha}\left(t^2 + 2(1-\cos t)w\right) \le -\frac{1}{2\alpha}(1+w)t^2. \tag{36}$$

The last line follows using the well known inequality $1 - \cos t \le t^2/2$ for all $t \in \mathbb{R}$ and the fact that $w < 0$. Thus, we have

$$\int_{|t|>\alpha^c} e^{f(t+z_0)}\mathrm{d}t \le e^{f(z_0)} \int_{|t|\ge\alpha^c} e^{\mathrm{Re}(f(t+z_0))-f(z_0)}\mathrm{d}t \le 2e^{f(z_0)} \int_{\alpha^c}^{\infty} e^{-(1+w)\alpha^{-1}t^2/2}\mathrm{d}t.$$

Again, since $w = o(1)$ the rightmost integral tends to zero faster than any power of α. Thus, we deduce that

$$\int_{-\infty}^{\infty} e^{f(t+z_0)}\mathrm{d}t \sim \sqrt{\frac{2\pi}{-f''(z_0)}}e^{f(z_0)}.$$

Therefore, from (10), we get $\phi(x,y) \sim e^{f(z_0)}$, which is equivalent to Part (a) of Proposition 4.

A.2 Part (b)

In this case, $\delta \in (-1, 0)$ is assumed to satisfy the condition $\alpha^{2/3} \ll |\delta| \ll 1 - \varepsilon$ for some fixed $\varepsilon > 0$. We proceed in the same manner as in the previous case, but since w can be very close to -1, $f''(z_0)$ can be small. We can still use the horizontal line passing through z_0 as our path of integration. However, this time, we do not ignore the term with $f'''(z_0)$ in the local integral. We choose $c \in (1/4, 1/3)$, and the Taylor approximation gives

$$f(t+z_0) = f(z_0) + f''(z_0)\frac{t^2}{2} + f'''(z_0)\frac{t^3}{6} + O(\alpha^{4c-1}),$$

uniformly for $|t| \le \alpha^c$. Thus,

$$\int_{-\alpha^c}^{\alpha^c} e^{f(t+z_0)}\mathrm{d}t = (1 + O(\alpha^{4c-1}))e^{f(z_0)} \int_{-\alpha^c}^{\alpha^c} e^{f''(z_0)t^2/2+f'''(z_0)t^3/6}\mathrm{d}t.$$

Let us denote the integral on the right-hand side by J. Making use of the values of $f''(z_0)$ and $f'''(z_0)$ in (33) and (34) respectively, and with the change of variable $t \mapsto \alpha^{1/3}t$, we can rewrite J in the following way:

$$J = 2\alpha^{1/3} \int_0^{\alpha^{c-1/3}} e^{-(1+w)\alpha^{-1/3}t^2/2} \cos\left(w\frac{t^3}{6}\right) \mathrm{d}t.$$

The term $1+w$ is always positive, and since $\delta \gg \alpha^{2/3}$, we can show from the asymptotic estimate (18) of the Lambert W function that $1+w \gg \alpha^{1/3}$. This implies that $(1+w)\alpha^{-1/3} \gg 1$. Adding the fact that $\alpha^{c-1/3} \to \infty$, we can extend the range of integration of J to infinity at the expense of a negligible error term. So we have

$$J \sim 2\alpha^{1/3} \int_0^{\infty} e^{-(1+w)\alpha^{-1/3}t^2/2} \cos\left(w\frac{t^3}{6}\right) \mathrm{d}t.$$

With an appropriate change of variable, the right-hand side can be written in terms of the Airy function $\mathrm{Ai}(z)$ (here we can use the integral representation of $\mathrm{Ai}(z)$ in [28, (9.5.7)]). Skipping the calculations, we have

$$J \sim 2^{4/3}\pi|w|^{-1/3}\alpha^{1/3}e^{2R^{3/2}/3}\mathrm{Ai}(R),$$

where $R = 2^{-2/3}(1+w)^2 w^{-4/3}\alpha^{-2/3}$.

Now for the estimates of the tail, we use the same argument as in the previous case. Inequality (36) is valid in this case as well, so we still have

$$\int_{|t|\geq\alpha^c} e^{f(t+z_0)}\mathrm{d}t \leq 2e^{f(z_0)} \int_{\alpha^c}^{\infty} e^{-(1+w)\alpha^{-1}t^2/2}\mathrm{d}t.$$

With $1+w \gg \alpha^{1/3}$ and $c > 1/3$ the integral on the right-hand side tends to zero faster than any power of α. Hence, the main contribution would come from the local integral if we can show that $e^{2R^{3/2}/3}\mathrm{Ai}(R)$ is bounded below by some power of α. But the definition of R given above guarantees that R is always positive, and it is bounded above by a function that is $O(\alpha^{-2/3})$. Hence, by the asymptotic formula of the Airy function $e^{2R^{3/2}/3}\mathrm{Ai}(R) \gg R^{-1/4} \gg \alpha^{-1/6}$. Therefore, we deduce that

$$\phi(x,y) \sim 2^{5/6}\pi^{1/2}|w|^{-1/3}\mathrm{Ai}(R)\alpha^{-1/6}e^{2R^{3/2}/3+f(z_0)}.$$

The latter gives the formula in Part (b) of Proposition 4.

A.3 Part (c)

This case is slightly different from the previous two. The saddle-point z_0 is too close to i so we choose the path of integration Γ shown in Figure 2. For the local integral, we consider up to the 5-th term in the Taylor approximation of the function $f(z)$ around i. We have $f'(i) = i\delta\alpha^{-1}$, $f''(i) = \delta\alpha^{-1}$, $f'''(i) = -i(1+\delta)\alpha^{-1}$ and $f^{(4)}(i) = -(1+\delta)\alpha^{-1}$. We choose $c \in (1/5, 1/3)$. For $|z-i| \leq \alpha^c$ and $z \in \Gamma$, we can write

$$e^{f(z)} = e^{f(i)+\mu_1(z-i)+\mu_3(z-i)^3}\left(1 + \zeta_2(z-i)^2 + \zeta_4(z-i)^4 + O(\alpha^{5c-1})\right),$$

where $\mu_1 = i\theta\alpha^{-1/3}$, $\mu_3 = -\frac{1}{6}i\alpha^{-1}$, $\zeta_2 = \frac{1}{2}\theta\alpha^{-1/3}$, $\zeta_4 = -\frac{1}{24}(1+\theta\alpha^{2/3})\alpha^{-1}$ (we used the fact that $\delta = \theta\alpha^{2/3}$). Let us denote by Γ_c the part of Γ that lies in the disk $|z-i| \leq \alpha^c$. For each integer $k \geq 0$, let

$$\mathcal{I}_k := \int_{\Gamma_c} (z-i)^k e^{\mu_1(z-i)+\mu_3(z-i)^3}\mathrm{d}z.$$

We parametrize Γ_c and show that the the two half-segments of Γ_c can be extended to ∞ with an error smaller than any power of α. Then, with some suitable change of variable, (skipping all details) we can express $\mathcal{I}_k$ in terms of the k-th derivative of the Airy function as follows

$$\mathcal{I}_k = -i^{k+2}\,\pi\,2^{(k+4)/3}(1+\delta)^{-(k+1)/3}\alpha^{(k+1)/3}\mathrm{Ai}^{(k)}(R) + \cdots$$

where by "$\cdots$" we mean an exponentially small term, and

$$R = i\mu_1(3i\mu_3)^{-1/3} = -2^{1/3}\delta(1+\delta)^{-1/3}\delta\alpha^{-2/3} = -2^{1/3}\theta\,(1+\delta)^{-1/3}.$$

Thus, we obtain

$$\begin{aligned}
\zeta_0\,\mathcal{I}_0 &= \pi\,2^{4/3}(1+\delta)^{-1/3}\alpha^{1/3}\mathrm{Ai}(R) + \cdots\\
\zeta_2\,\mathcal{I}_2 &= -2\pi\theta\,(1+\delta)^{-1}\alpha^{2/3}\mathrm{Ai}^{(2)}(R) + \cdots\\
\zeta_4\,\mathcal{I}_4 &= -\tfrac{1}{3}\pi\,2^{-1/3}(1+\delta)^{-2/3}\alpha^{2/3}\mathrm{Ai}^{(4)}(R) + \cdots
\end{aligned}$$

The higher derivatives of the Airy function can be written in terms of $\mathrm{Ai}(z)$ and $\mathrm{Ai}'(z)$ using the well known Airy differential equation as we can easily show by induction on k that

$$\mathrm{Ai}^{(k+3)}(z) = (k+1)\,\mathrm{Ai}^{(k)}(z) + z\,\mathrm{Ai}^{(k+1)}(z) \;\text{ for }\; k \geq 0.$$

Reducing all higher derivatives of the Airy function and using Taylor approximation to estimate each of the $\mathrm{Ai}^{(k)}(R)$'s, we get

$$\int_{\Gamma_c} e^{f(z)}\mathrm{d}z \sim e^{f(i)}\Big(K_1(\theta)\,\alpha^{1/3} + K_2(\theta)\,\alpha^{2/3} + O(\alpha)\Big),$$

where $K_1(\theta)$ and $K_2(\theta)$ are precisely as defined in Proposition 4.

Now we estimate the contribution of the tail. First, if t is real and $|t| \geq \sqrt{3}$, then we have

$$\mathrm{Re}(f(t)) - f(i) = -\frac{1}{2\alpha}(t^2-1) - \frac{\cos t}{e\alpha} + \frac{\delta}{\alpha}\Big(1 - \frac{\cos t}{e}\Big) \leq -\frac{|t|}{2\alpha}\Big(1 + O(\alpha^{2/3})\Big),$$

where the constant in the O term is independent of t. The inequality follows from the fact that if $|t| \geq \sqrt{3}$ then we have $((t^2-1)/2 - \cos(t)/e) \leq 0.5|t|$, which is not too difficult to verify. The above estimate is enough to show that the contribution from the real half-lines $|t| \geq \sqrt{3}$ is negligible.

If $z = i + te^{i\pi/6}$ and $t \in [-2, -\alpha^c]\}$, then we let $\xi(t) = 2e^{t/2}\cos(\sqrt{3}t/2)$ so that we have

$$\mathrm{Re}(f(i + te^{\pi i/6})) - f(i) = -\frac{1}{2\alpha}\Big(\xi(t) - 2 - t + \frac{t^2}{2} + \delta\;(\xi(t) - 2)\Big).$$

We can show (e.g., using a Taylor approximation of $\xi(t)$) that there exist positive absolute constants C_1 and C_2 such that $|\xi(t) - 2| \leq C_1|t|$ and $\xi(t) - 2 - t + \frac{t^2}{2} \geq C_2|t|^3$, for any $t \in [-2, 0]$. Hence, uniformly for $t \in [-2, -\alpha^c]$,

$$\mathrm{Re}(f(i + te^{\pi i/6})) - f(i) \leq -\frac{1}{2\alpha}\Big(C_2|t|^3 + O(\alpha^{2/3}|t|)\Big) \leq -C_2\frac{|t|^3}{2\alpha}(1 + O(\alpha^{2/3-2c})).$$

In particular, $\mathrm{Re}(f(i+te^{\pi i/6})) - f(i)$ is negative for sufficiently small α and $|\mathrm{Re}(f(i+te^{\pi i/6})) - f(i)| \gg \alpha^{3c-1}$ uniformly for $t \in [-2, -\alpha^c]$. This is enough to show that the contribution from the segment $\{i + te^{i\pi/6} \;:\; t \in [-2, -\alpha^c]\}$ is also negligible. The contribution from the segment $\{i + te^{-i\pi/6} \;:\; t \in [\alpha^c,\; 2]\}$ can also be dealt with in the same way.

B Idea of the Proof of Proposition 7

We are unable to give much detail here due to lack of space. But the proof of Proposition 7 is essentially the same as the one above. The main difference is, of course, that x is complex. Let $x = (1+\delta)x_0e^{iu}$ where $u \in (-\pi, \pi]$, $\delta = \theta\alpha^{2/3}$ and θ is a fixed number that satisfies $\mathrm{Ai}(-2^{1/3}\theta) \neq 0$. This implies that the number w, which is now defined as $W_0(-(1+\delta)e^{iu-1})$, is no longer real.

The proof of Part (c) above proceeds in essentially the same way as δ and u are both $O(\alpha^{2/3})$. But for Part (a) and Part (b) to work, we need the following result about w.

▶ **Lemma 10.** *The functions* $\mathrm{Re}((1+w)^2)$, $\mathrm{Re}(1+w)$ *and* $1-|w|$ *are all positive and nonzero if u is bounded away from 0. Moreover, if* $|u| \to 0$ *as* $\alpha \to 0^+$, *but* $|u| \gg \alpha^{2/3}$, *then*

$$w = -1 + \alpha^{1/3}\sqrt{-2(\theta+it)} + \frac{2}{3}\alpha^{2/3}(\theta+it) + O(|u|^{3/2}), \tag{37}$$

where $t = u\alpha^{-2/3}$, *and the implied constant does not depend on u. In particular, we have* $\mathrm{Re}(1+w) \gg \alpha^{1/3}$ *uniformly for* $\alpha^{2/3} \ll |u| \leq \pi$.

Proof. The asymptotic formula (37) follows easily from (18). Now to show that $\mathrm{Re}(1+w)$ and $1-|w|$ stay positive, we just need to show that this is the case for $1-|w|$ since $\mathrm{Re}(1+w) \geq 1-|w|$.

If $|w| = 1$, then from the definition of w we have

$$|w|e^{\mathrm{Re}(1+w)} = e^{\mathrm{Re}(1+w)} = 1 + O(\alpha^{2/3}).$$

This implies that $\mathrm{Re}(1+w) \to 0$, which means $w = -1 + o(1)$. The latter forces u to tend to zero.

Similarly if $\mathrm{Re}((1+w)^2) = 0$, then w must be of the form $w = -1 + a(1 \pm i)$, where $a \in \mathbb{R}$. This implies that

$$|w|e^{\mathrm{Re}(1+w)} = \sqrt{a^2 + (a-1)^2}\, e^a = 1 + O(\alpha^{2/3}).$$

This is only possible if $a \to 0$ as $\alpha \to 0$. ◀

This lemma will be very useful in proving Part (a) and Part (b). It shows, for example, that $\mathrm{Re}(-f''(z_0))$ is positive and it satisfies $\mathrm{Re}(-f''(z_0)) = \mathrm{Re}((1+w)\alpha^{-1}) \gg \alpha^{-2/3}$ uniformly for $\alpha^{2/3} \ll |u| \leq \pi$. This will make the proofs of Part (a) and Part (b) above work in this case as well.