Local Approximations of the Independent Set Polynomial

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Abstract

The independent set polynomial of a graph has one variable for each vertex and one monomial for each independent set, comprising the product of the corresponding variables. Given a graph G on n vertices and a vector $\boldsymbol{p} \in [0,1)^n$, a central problem in statistical mechanics is determining whether the independent set polynomial of G is non-vanishing in the polydisk of $\boldsymbol{p}$, i.e., whether $|Z_G(\boldsymbol{x})| > 0$ for every $\boldsymbol{x} \in \mathbb{C}^n$ such that $|x_i| \le p_i$. Remarkably, when this holds, $Z_G(-\boldsymbol{p})$ is a lower bound for the avoidance probability when G is a dependency graph for n events whose probabilities form vector $\boldsymbol{p}$. A *local* sufficient condition for $|Z_G| > 0$ in the polydisk of $\boldsymbol{p}$ is the Lovász Local Lemma (LLL).

In this work we derive several new results on the efficient evaluation and bounding of Z_G. Our starting point is a monotone mapping from subgraphs of G to truncations of the tree of self-avoiding walks of G. Using this mapping our first result is a local *upper* bound for $Z(-\boldsymbol{p})$, similar in spirit to the local lower bound for $Z(-\boldsymbol{p})$ provided by the LLL. Next, using this mapping, we show that when G is chordal, Z_G can be computed exactly and in linear time on the entire complex plane, implying *perfect* sampling for the hard-core model on chordal graphs. We also revisit the task of bounding $Z(-\boldsymbol{p})$ from below, i.e., the LLL setting, and derive four new lower bounds of increasing sophistication. Already our simplest (and weakest) bound yields a strict improvement of the famous asymmetric LLL, i.e., a strict relaxation of the inequalities of the asymmetric LLL without any further assumptions. This new asymmetric local lemma is sharp enough to recover Shearer's *optimal* bound in terms of the maximum degree $\Delta(G)$. We also apply our more sophisticated bounds to estimate the zero-free region of the hard-core model on the triangular lattice (hard hexagons model).

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1 The Independent Set Polynomial

We write $[n]$ to denote the set $\{1, 2, \ldots, n\}$, with the convention $[0] = \emptyset$. Throughout, G is a graph on $[n]$ and $\mathrm{Ind}(G)$ denotes the set of all independent sets of G.

▶ **Definition 1.** *The* independent set polynomial *of a graph G with variables $x_1, \ldots, x_n$ is*

$$Z_G(\boldsymbol{x}) = Z(\boldsymbol{x}) := \sum_{\substack{I \subseteq S \\ I \in \mathrm{Ind}(G)}} \prod_{i \in I} x_i \quad . \tag{1}$$

For arbitrary $S \subseteq [n]$ we denote the independent set polynomial of the subgraph of G induced by S by $Z_G(\boldsymbol{x}; S) = Z(S)$, the latter notation relying on $\boldsymbol{x}$ being clear from context.

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► Remark 2. We will often refer to the components of the variable vector $\boldsymbol{x}$ as *activities*.

► **Definition 3.** *The* polydisk *of* $\boldsymbol{p} \in [0,\infty)^n$ *is the set* $\{\boldsymbol{x} \in \mathbb{C}^n : |x_i| \le p_i$ *for all* $i \in [n]\}$.

The complexity of computing and approximating the independent set polynomial is an extensively studied subject. This is because there are important instantiations of the polynomial when the activities are positive reals, negative reals, and even complex numbers.

1.1 Positive Reals: The Hard-Core Model

In many natural computational problems in combinatorics, statistics, and statistical physics we are given as input a graph G that defines a set $\Omega = \Omega(G)$ of objects (configurations) of interest, e.g., matchings in G. A weight function $w : \Omega \to (0,+\infty)$ assigns a positive weight to each element $\sigma \in \Omega$, giving rise to a probability distribution $\pi(\sigma) = w(\sigma)/Z$, where the normalizing factor $Z := \sum_{\sigma\in\Omega} w(\sigma)$ is called the *partition function.* When $\Omega = \mathrm{Ind}(G)$ and each $I \in \mathrm{Ind}(G)$ has weight $w(I) = \prod_{i\in I} x_i$, where $\boldsymbol{x} \in (0,+\infty)^n$, the distribution is the *hard-core* model of statistical physics, and the independent set polynomial when $S = [n]$ equals its partition function. Observe that in the *univariate* case where all vertex activities equal $x > 0$, i.e., $\boldsymbol{x} = x\mathbf{1}$, as $x \to \infty$ the polynomial is increasingly dominated by the contribution of the largest independent sets, readily suggesting the intractability of evaluating the polynomial for arbitrarily large values of x. A celebrated achievement in this area is the characterization of the computational tractability of approximating the univariate partition function. Let $\Delta = \Delta(G)$ denote the maximum degree of G, let $\boldsymbol{x} = x\mathbf{1}$, and let

$$x_c = x_c(\Delta) := \frac{(\Delta-1)^{\Delta-1}}{(\Delta-2)^{\Delta}} \searrow \frac{\mathrm{e}}{\Delta} \ ,$$

where $\searrow$ denotes convergence from above. Weitz [22] proved the partition function can be approximated arbitrary well (FPTAS) for $x < x_c$, while Sly and Sun [19] proved that approximating the partition function is NP-hard for $x > x_c$.

1.2 Complex Numbers: Phase Transitions

The study of partition functions when the arguments of the corresponding polynomial are complex numbers dates back to the 1952 work of Lee and Yang [23] who established a connection between the location of zeros of the partition function on the complex plane and the presence of phase transitions on the real axis. The high-level idea is that since we identify phase transitions as discontinuities in the derivatives of free energy, i.e., of $\log Z$, such a transition can only occur at a point of the complex plane if there is at least one nearby zero of the partition function. Specifically, in the follow-up paper [12], Lee and Yang instantiated this connection for the ferromagnetic Ising model by proving that the zeros of the partition function always lie on the unit circle in the complex plane, and used this fact to conclude that the ferromagnetic Ising model can have at most one phase transition. The Lee-Yang approach has since become a cornerstone of the study of phase transitions, and has been used extensively in the statistical physics literature: see, e.g., [2, 9, 13, 21] for specific examples, and Ruelle's book [16] for background. There have also been attempts to relate the Lee-Yang program to the Riemann hypothesis [14].

Zeros of partition functions when the variables take complex values have also been studied in a purely combinatorial setting without reference to the physical interpretation: see, for example, Choe et al. [6]. Another important example is the work of Chudnovsky and Seymour [7], who show that the zeros of the univariate independent set polynomial of claw-free graphs lie on the real line. Finally, in a seminal work, Scott and Sokal [17] proved that the independent set polynomial is non-zero in the polydisk of $\boldsymbol{p} \in [0,1)^n$, if and only if $Z_G(-\lambda \boldsymbol{p}) > 0$ for every $\lambda \in [0,1]$.

1.3 The Probabilistic Method and the Lovász Local Lemma

The *Probabilistic Method* [1] amounts to establishing the existence of mathematical objects with a property of interest by demonstrating a probability distribution under which they have positive probability. The power of the method stems from the fact that if the probability of the objects under the distribution is indeed positive, then *any* multiplicative underestimation of it is enough to imply existence. Typically, the property of interest, $\mathcal{P}$, is the intersection of the complements of several simpler properties, each property expressing some particular "flaw," so that $\mathcal{P}$ coincides with flawlessness. Thus, if we endow a universe of candidate objects Ω, where sets $\{F_i\}_{i=1}^n \subseteq \Omega$ correspond to the different flaws, with a probability measure μ, the goal is to prove that the *avoidance probability*, $\mu(\bigcap_{i \in [n]} \overline{F}_i)$, is strictly positive.

Given only the marginals $p_i := \mu(F_i)$, the best lower bound we can give for the avoidance probability is $1 - \sum_i p_i$ since, for all we know, the flaws could be disjoint. To improve upon the union bound, we need to constrain the flaw overlaps. A natural and extremely successful way to do this is in terms of a graph G on $[n]$. Concretely, let $\Gamma_i(G) = \Gamma_i$ denote the neighborhood of vertex i in G and let $\Gamma_i^+ = \Gamma_i \cup \{i\}$. We say that G is a *dependency graph* for $\{F_i\}_{i=1}^n$ with respect to μ if for every $i \in [n]$ and every set $\{j_1, j_2, \ldots\} \subseteq [n] \setminus \Gamma_i^+$,

$$\mu(F_i \mid \overline{F_{j_1}} \cap \overline{F_{j_2}} \cap \cdots) = \mu(F_i) = p_i \quad . \tag{2}$$

Note that the presence of an edge in G does not prescribe any specific kind of dependency between its two corresponding events, only a lack of constraint thereof. Thus, a complete dependency graph (clique) conveys no information at all about how the n events overlap, while an empty dependency graph implies that the n events are mutually independent.

In applications, given the measure μ and the sets of flaws $\{F_i\}_{i=1}^n$ it is typically difficult to derive much more than a vector $\boldsymbol{p} = (p_1, p_2, \ldots, p_n)$ of (upper bounds for) the flaw probabilities and a (possibly pessimistic) dependency graph G. As a result, it is desirable to have sufficient conditions for a pair $\boldsymbol{p}, G$ to have the property that *every* probability measure compatible with it has strictly positive avoidance probability. Remarkably, Shearer [18] gave a sufficient *and necessary* condition for a pair to have this property.

▶ **Definition 4.** *Given a graph G, let $\mathcal{S}(G) = \{\boldsymbol{p} \in [0,1)^n : Z_G(-\boldsymbol{p}; S) > 0$, for all $S \subseteq [n]\}$.*

Shearer showed that membership in $\mathcal{S}(G)$ characterizes the vectors $\boldsymbol{p}$ for which every probability measure compatible with $\boldsymbol{p}, G$ has strictly positive avoidance probability. For this he showed that given $\boldsymbol{p}, G$, in order to minimize the avoidance probability, one should try to realize the (unique) measure μ^* under which events adjacent in G are disjoint. He then showed that if $Z(-\boldsymbol{p}; S) \le 0$ for some $S \subseteq [n]$, then μ^* can not be realized and the avoidance probability is 0, while, otherwise, $\mu^*(\bigcap_{i \in S} \overline{F}_i) = Z(-\boldsymbol{p}; S) \ge 0$ for every $S \subseteq [n]$ and, therefore, the avoidance probability is at least $Z(-\boldsymbol{p}; [n])$, i.e., the value of the independent set polynomial of G at $-\boldsymbol{p}$. Unfortunately, performing this evaluation is generally intractable, as it involves a summation over $\mathrm{Ind}(G)$.

The Lovász Local Lemma is a *sufficient* condition for membership in $\mathcal{S}(G)$, along with a lower bound for $Z(-\boldsymbol{p})$. Below is a general formulation (the so-called *asymmetric*).

▶ **Theorem 5** (Lovász [20]). *Let μ be a probability measure on set Ω and let G be a dependency graph for $\{F_i\}_{i\in[n]} \subseteq \Omega$. If there exist $r_1, r_2, \ldots, r_n \in [0,1)$ such that for every $i \in [n]$,*

$$p_i \leq r_i \prod_{j\in\Gamma_i} (1-r_j) \ , \tag{3}$$

then $\mu\left(\bigcap_{i=1}^{n} \overline{F_i}\right) \geq \prod_{i\in[n]} (1-r_i) > 0.$

▶ Remark 6. Theorem 5 holds (and is known as the "Lopsided LLL" of Erdős and Spencer [8]) if condition (2) holds with "$\leq$" instead of "$=$". All our results also hold in that setting.

2 Our Results

2.1 An Improved General / Asymmetric LLL

We strictly improve the asymmetric LLL, and thus all its applications, as follows.

▶ **Theorem 7.** *Theorem 5 holds if (3) is replaced by*

$$p_i \leq r_i \prod_{j\in\Gamma_i} \frac{1-r_j}{1-r_i r_j} \ . \tag{4}$$

While our Theorem 7 retains all the flexibility of the asymmetric LLL to adjust to events with different degrees and probabilities, it is sharp enough to recover the *optimal* bound in terms of the maximum degree $\Delta(G)$ (attained as a limit by Δ-regular trees as depth goes to infinity). Specifically, if every event has probability at most p and is mutually independent of all but $\Delta \geq 2$ other events, Theorem 7 implies the optimal condition $p < \frac{(\Delta-1)^{(\Delta-1)}}{\Delta^{\Delta}}$ originally proven by Shearer [18], whereas the asymmetric LLL requires $p < \frac{\Delta^{\Delta}}{(\Delta+1)^{(\Delta+1)}}$.

A fairly recent improvement of Theorem 5 is the so-called *cluster expansion* LLL by Bissacot et al. [5], wherein the presence of edges in the neighborhood of a vertex, i.e., the presence of triangles, allow one to relax the condition corresponding to that vertex. While our Theorem 7 is, in general, incomparable with the cluster expansion LLL, the overall trend is that the former wins when neighborhoods are sparse, while the latter when they are dense.

In Sections 2.4, 2.5 we will see four significant improvements of Theorem 7. The weakest of these is already *exact* on *arbitrary* trees (uniform trees being the worst case for given Δ).

2.2 An Upper Bound for the Partition Function on the Negative Reals

Recall that given a vector $\boldsymbol{p}$, the central problem is determining whether $|Z_G| > 0$ on the *polydisk* of $\boldsymbol{p}$, i.e., for every $\boldsymbol{x} \in \mathbb{C}^n$ such that $|x_i| \leq p_i$ for all $i \in [n]$. Since $Z_G(\mathbf{0}) = 1 > 0$, if $\boldsymbol{p} \notin \mathcal{S}(G)$, continuity implies $|Z_G(\lambda \boldsymbol{p}_S)| = 0$ for some $S \subseteq [n]$ and $\lambda \in (0,1]$, where $\boldsymbol{p}_S$ is the vector that results by setting to 0 all coordinates of $\boldsymbol{p}$ outside S. On the other hand, Scott and Sokal [17] showed that for $\boldsymbol{p} \in \mathcal{S}(G)$ and every $\lambda \in [0,1]$, the magnitude of Z_G over the polydisk of $\lambda\boldsymbol{p}$ is minimized at $-\lambda\boldsymbol{p}$. Thus, membership in $\mathcal{S}(G)$ is equivalent to $Z(-\lambda\boldsymbol{p}) > 0$ for every $\lambda \in [0,1]$ and characterizes the vectors on whose polydisks Z_G does not vanish.

The LLL is a local sufficient condition for $\boldsymbol{p} \in \mathcal{S}(G)$, providing a strictly positive lower bound for $Z_G(-\boldsymbol{p})$ for such $\boldsymbol{p}$ (and, thus, for $|Z_G|$ on the polydisk of $\boldsymbol{p}$). We show that $Z_G(-\boldsymbol{p})$ can also be bounded *from above* for $\boldsymbol{p} \in \mathcal{S}(G)$.

▶ **Definition 8.** *Given a permutation π of $[n]$, let $\overleftarrow{\Gamma_i} = \overleftarrow{\Gamma_i}(\pi) = \Gamma_i \cap \{j \in [n] : \pi(j) < \pi(i)\}$ and let $\overrightarrow{\Gamma_i} = \overrightarrow{\Gamma_i}(\pi) = \Gamma_i \cap \{j \in [n] : \pi(j) > \pi(i)\}$.*

▶ **Theorem 9** (Upper Bound). *Given $\boldsymbol{p}, G$ and a permutation π of $[n]$, define $\boldsymbol{r} = \boldsymbol{r}(\pi)$ by*

$$p_i = r_i \prod_{j \in \overleftarrow{\Gamma}_i(\pi)} (1 - r_j) \ , \quad \text{for every } i \in [n] \ . \tag{5}$$

(Note that $\boldsymbol{r}$ is well-defined as $r_1 = p_1$, while for $i > 1$, r_i is determined by $p_i, r_1, \ldots, r_{i-1}$.)

If $\boldsymbol{p} \in \mathcal{S}(G)$, then $Z(-\boldsymbol{p}; S) \le \prod_{j \in S}(1 - r_j)$, for every $S \subseteq [n]$.

▶ Remark 10. If $\boldsymbol{r'}$ satisfies (3) and $\boldsymbol{r}$ is defined by (5), then $1 - r'_i \le 1 - r_i$ for every $i \in [n]$.

2.3 Exact Partition Function Computation for Chordal Graphs

Recall that a graph is *chordal* if all its induced cycles have length three. We prove that the independent set polynomial of a chordal graph can be evaluated *anywhere* on the complex plane in *linear* time. We conjecture that chordality is closely related to the exact solvability of the hard-core model for certain highly transitive graphs, e.g., triangular lattice (hard hexagons model [3]), and that the hard-core model is not the only statistical mechanics model for which chordality relates to exact solvability. We leave this as future work.

▶ **Fact 11.** *A graph G on $[n]$ is chordal iff it has a* perfect elimination ordering*, i.e., a permutation π of $[n]$ such that $\overrightarrow{\Gamma}_i(\pi)$ is a clique for every $i \in [n]$. If the identity permutation is a perfect elimination ordering for G, we say that G is chordally presented.*

▶ **Theorem 12.** *If G is chordally presented, then $Z_G(\boldsymbol{x}) = \prod_{i \in [n]} (1 + r_i)$, where*

$$x_i = r_i \prod_{j \in \overleftarrow{\Gamma}_i} (1 + r_j) \ , \quad \text{for every } i \in [n] \ . \tag{6}$$

(Note that $\boldsymbol{r}$ is well-defined as $r_1 = x_1$, while for $i > 1$, r_i is determined by $x_i, r_1, \ldots, r_{i-1}$.)

▶ **Corollary 13.** *The independent set polynomial of a chordal graph can be evaluated anywhere on the complex plane in linear time. A perfect sample from the hard-core distribution on a chordal graph can be obtained in linear time.*

Proof. A chordal presentation of chordal graph $G = (V, E)$ can be found in time $O(|V| + |E|)$. Computing each r_i given $r_1, \ldots, r_{i-1}$ requires $O(|\Gamma_i|)$ steps. Thus, $Z_G(\boldsymbol{x}, [n])$ can be evaluated in $O(|V| + |E|)$ steps. Regarding sampling we observe that chordal graphs are closed with respect to vertex deletions. Thus, given $Z_G(\boldsymbol{x}, S)$ for arbitrary $S \subseteq [n]$ and $\{r_i\}_{i \in S}$, computing $Z_G(\boldsymbol{x}, T)$ for $T \subseteq S$ can be done by $O(|S| - |T|)$ divisions. Since $\{r_i\}_{i \in [n]}$ can be computed in $O(|V| + |E|)$ steps via (6), the claim follows. ◀

The previous best result on the independent set polynomial of chordal graphs is due to Okamoto, Uno, and Uehara [15] who showed that it can be evaluated exactly in linear time at $\boldsymbol{x} = \boldsymbol{1}$, i.e., that the number of independent sets can be counted. Since their algorithm is also capable of counting the number of independent sets of any given size $k = 1, \ldots, n$ in linear time, evaluating the univariate independent set polynomial can be done in polynomial time. However, our algorithm is significantly simpler, runs in linear time, and works also on the multivariate setting. A very recent related work by Heinrich and Müller [10] showed that the independent set polynomial can be evaluated exactly for $\boldsymbol{x} \in \mathbb{R}^n$, when G is strongly orderable. These form a subclass of weakly chordal graphs that contains chordal bipartite graphs. Finally, in terms of (arbitrarily good, randomized) approximate evaluation of the independent set polynomial, Bezakova and Sun [4] showed that a natural Markov chain for the hard core model with positive fugacities, i.e., for the case $\boldsymbol{x} \in \mathbb{R}^n$, mixes in polynomial time on chordal graphs with separators of *bounded* size.

2.4 Local Lemmata on Unordered Vertices (Simpler)

In this section we present four local lemmata providing sufficient conditions for $\boldsymbol{p} \in \mathcal{S}(G)$. As we will see in Section 3.2, determining $Z_G(-\boldsymbol{p})$ exactly amounts to understanding the set of all possible walks on G obeying certain ordering and self-avoidance constraints.

Dropping the ordering restriction and replacing self-avoidance by non-repetitiveness within distance 1 gives Theorem 14. Extending the scope of non-repetitiveness to distance 2 gives Theorem 15. Enforcing the ordering restriction while replacing self-avoidance by non-repetitiveness within distance 1 and 2, yields Theorems 17 and 18, respectively.

2.4.1 Incorporating All Paths of Length at most One

▶ **Theorem 14.** *Given $\boldsymbol{p} \in [0,1)^n$ and G, assume that for every path (i) of length 0 and every path (i,j) of length 1, there exist $r_i, r_{i,j} \in [0,1)$, respectively, such that*

$$p_i \leq r_i \prod_{j \in \Gamma_i} (1 - r_{i,j}) \tag{7}$$

$$p_j \leq r_{i,j} \prod_{k \in \Gamma_j \setminus \{i\}} (1 - r_{j,k}) \ . \tag{8}$$

Then, $Z(-\boldsymbol{p}) \geq \prod_{i \in [n]} (1 - r_i)$.

Theorem 7 follows from Theorem 14, as we show in Section 4.3: given $\{r'_i\}_{i \in [n]}$ satisfying (4) we can compute $r_{i,j}$ for every oriented edge (i,j) to satisfy (7), (8) (with $r_i = r'_i$).

2.4.2 Incorporating All Paths of Length at most Two

▶ **Theorem 15.** *Given $\boldsymbol{p} \in [0,1)^n$ and G, assume that for every path (i) of length 0, every path (i,j) of length 1, and every path (i,j,k) of length 2 such that $i \in \Gamma_k$, there exist $r_i, r_{i,j}, r_{i,j,k} \in [0,1)$, respectively, such that*

$$p_i \leq r_i \prod_{j \in \Gamma_i} (1 - r_{i,j}) \tag{9}$$

$$p_j \leq r_{i,j} \prod_{\substack{k \in \Gamma_j \setminus \{i\} \\ i \notin \Gamma_k}} (1 - r_{j,k}) \prod_{\substack{k \in \Gamma_j \setminus \{i\} \\ i \in \Gamma_k}} (1 - r_{i,j,k}) \tag{10}$$

$$p_k \leq r_{i,j,k} \prod_{\substack{\ell \in \Gamma_k \setminus \{i,j\} \\ j \notin \Gamma_\ell}} (1 - r_{k,\ell}) \prod_{\substack{\ell \in \Gamma_k \setminus \{i,j\} \\ j \in \Gamma_\ell}} (1 - r_{j,k,\ell}) \ . \tag{11}$$

Then, $Z(-\boldsymbol{p}) \geq \prod_{i \in [n]} (1 - r_i)$.

2.5 Local Lemmata on Ordered Vertices (Sharper)

A *walk* starting at vertex i is a sequence of vertices $(v_0, v_1, \ldots, v_\ell)$, such that $v_0 = i$ and for all $k \in [\ell]$, vertex v_{k-1} is adjacent to vertex v_k.

▶ **Definition 16.** *Given a walk $w = (v_0, v_1, \ldots, v_\ell)$, let $\mathcal{F}(v_0) = \emptyset$, while for $k \in [\ell]$ let*

$$\mathcal{F}(v_0, \ldots, v_k) = \mathcal{F}(v_0, \ldots, v_{k-1}) \cup \{v_{k-1}\} \cup \{u \in \Gamma_{v_{k-1}} : u \geq v_k\} \ . \tag{12}$$

Let $\mathcal{N}(v_0, \ldots, v_\ell) = \Gamma_{v_\ell} \cap \mathcal{F}(v_0, \ldots, v_\ell)$.

2.5.1 Incorporating All Paths of Length at most One

▶ **Theorem 17.** *Given $\boldsymbol{p} \in [0,1)^n$ and G, assume that for every vertex $i \in [n]$ and every oriented edge (i,j) there exist $r_i, r_{i,j} \in [0,1)$, respectively, such that*

$$p_i \leq r_i \prod_{j \in \Gamma_i} (1 - r_{i,j}) \tag{13}$$

$$p_j \leq r_{i,j} \prod_{k \in \Gamma_j \setminus \mathcal{N}(i,j)} (1 - r_{j,k}) \ . \tag{14}$$

Then, $Z(-\boldsymbol{p}) \geq \prod_{i \in [n]}(1 - r_i)$.

Theorem 17 implies Theorem 14, since $\{i\} \subseteq \mathcal{N}(i,j)$ implying that any collection of numbers satisfying (8) also satisfies (14).

2.5.2 Incorporating All Paths of Length at most Two

▶ **Theorem 18.** *Given $\boldsymbol{p} \in [0,1)^n$ and G assume that for every path (i) of length 0, every path (i,j) of length 1, and every path (i,j,k) of length 2 for which $\mathcal{N}(i,j,k) \neq \mathcal{N}(j,k)$, there exist $r_i, r_{i,j}, r_{i,j,k} \in [0,1)$, respectively, such that*

$$p_i \leq r_i \prod_{j \in \Gamma_i} (1 - r_{i,j}) \tag{15}$$

$$p_j \leq r_{i,j} \prod_{\substack{k \in \Gamma_j \setminus \mathcal{N}(i,j) \\ \mathcal{N}(i,j,k) = \mathcal{N}(j,k)}} (1 - r_{j,k}) \prod_{\substack{k \in \Gamma_j \setminus \mathcal{N}(i,j) \\ \mathcal{N}(i,j,k) \neq \mathcal{N}(j,k)}} (1 - r_{i,j,k}) \tag{16}$$

$$p_k \leq r_{i,j,k} \prod_{\substack{\ell \in \Gamma_k \setminus \mathcal{N}(i,j,k) \\ \mathcal{N}(j,k,\ell) = \mathcal{N}(k,\ell)}} (1 - r_{k,\ell}) \prod_{\substack{\ell \in \Gamma_k \setminus \mathcal{N}(i,j,k) \\ \mathcal{N}(j,k,\ell) \neq \mathcal{N}(k,\ell)}} (1 - r_{j,k,\ell}) \ . \tag{17}$$

Then, $Z(-\boldsymbol{p}) \geq \prod_{i \in [n]}(1 - r_i)$.

Theorem 18 implies Theorem 15, since $\{i\} \subseteq \mathcal{N}(i,j)$ and $\Gamma_k \cap \{i,j\} \subseteq \mathcal{N}(i,j,k)$, implying that any collection of numbers satisfying (10), (11) also satisfy (16), (17).

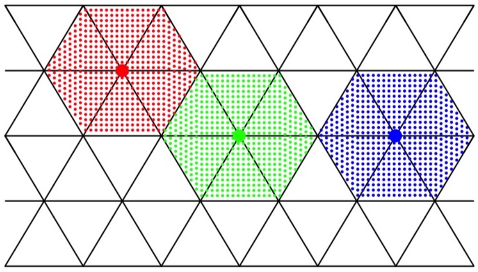
Theorem 18 also yields Theorem 17, by replacing the set $\mathcal{N}(i,j,k)$ in inequality (17) with its subset $\mathcal{N}(i,j)$ and imposing the additional equality constraints $r_{i,j,k} = r_{j,k}$. These modifications increase the number of (shrinking) factors in both (16) and (17), and together with the additional equality constraints make the resulting system of inequalities stricter.

Thus, to prove Theorems 14–18 it suffices to prove Theorem 18, which we do in Section 4.4.

2.6 Benchmarking: the Radii of $\mathcal{S}(G)$

As mentioned earlier, determining the set of activities for which the partition function is non-vanishing in the corresponding polydisk is a central problem in statistical mechanics. This is primarily motivated by the Lee-Yang [23] approach to studying phase transitions. Since phase transitions (non-analyticities of [one or more derivatives of] the log-partition function) can occur only in infinite-size systems, to study them on a locally-finite countable graph G_∞ (typically a regular lattice), we consider an increasing sequence of subgraphs $(G_n)_{n \geq 1}$ converging to G_∞ and study the limiting free energy per vertex $f_{G_\infty} = \lim_{n \to \infty} n^{-1} \log Z_{G_n}(\boldsymbol{x})$. Nonanalyticities of f_{G_∞} for real $\boldsymbol{x}$, arise from singularities of $\log Z_{G_n}(\boldsymbol{x})$ for complex $\boldsymbol{x}$ that approach the real axis in the limit $n \to \infty$. But the singularities of $\log Z_{G_n}(\boldsymbol{x})$ are precisely the zeros of $Z_{G_n}(\boldsymbol{x})$, hence the desire to determine the set $\mathcal{S}(G)$. Of particular interest is the so-called *uniform*, i.e., univariate, case $\boldsymbol{x} = x\mathbf{1}$, where all the activities are the same.

To benchmark our methods, we consider one of the very few exactly solved cases of the hard-core model, namely the case where G_∞ is the triangular lattice. This is known as the "hard hegaxons" model, since its valid configurations amount to placements of (centers of) hexagons in a triangular lattice so that no two hexagons overlap, i.e., to selecting an independent set of the triangular lattice to serve as the set of hexagon centers.



For this model it is known that the critical value is $x_c = \frac{5\sqrt{5}-11}{2} = 0.09016...$ Applying the asymmetric LLL, which only exploits that $\Delta(G_n) = 6$, gives $x_c \geq \Delta^\Delta/(\Delta+1)^{\Delta+1} = 6^6/7^7 = 0.0566$. Our improved asymmetric LLL (Theorem 7), improving the dependence on Δ, yields $x_c \geq (\Delta-1)^{\Delta-1}/\Delta^\Delta = 5^5/6^6 = 0.0669$.

Kolipaka, Szegedy, and Xu [11], introduced a family of sufficient conditions for the avoidance probability to be positive that range between the asymmetric LLL and the exact result of Shearer [18]. To apply their so-called "clique LLL" we color the triangular faces in a chess board pattern and decompose the triangular lattice using the white triangles as the parts of the clique-decomposition. Optimizing the resulting parameters yields $x_c \geq 0.07407$.

Finally, the cluster expansion LLL of Bissacot et al. [5], exploiting the presence of 6 triangles in the neighborhood of each vertex, yields $x_c \geq 0.0776$.

2.6.1 Simpler Bound: $x_c \geq 0.08115$

To apply Theorem 17 in the triangular lattice we order the neighbors of each vertex by taking the eastern neighbor to be the greatest, and then descending counter-clockwise. The translation symmetry of the lattice allows us to capture all possible paths of length up to one using only seven variables. Specifically, r_0 corresponds to vertices (paths of length 0), r_1 corresponds to arcs (paths of length 1) heading east, r_2 to arcs heading northeast, etc. Thus, inequalities (13) and (14) require x to be simultaneously less than all of the following:

$$r_0 \cdot (1-r_1) \cdot (1-r_2) \cdot (1-r_3) \cdot (1-r_4) \cdot (1-r_5) \cdot (1-r_6)$$
$$r_1 \cdot (1-r_1) \cdot (1-r_2) \cdot (1-r_3) \cdot (1-r_5) \cdot (1-r_6)$$
$$r_2 \cdot (1-r_1) \cdot (1-r_2) \cdot (1-r_3) \cdot (1-r_4)$$
$$r_3 \cdot (1-r_2) \cdot (1-r_3) \cdot (1-r_4) \cdot (1-r_5)$$
$$r_4 \cdot (1-r_3) \cdot (1-r_4) \cdot (1-r_5) \cdot (1-r_6)$$
$$r_5 \cdot (1-r_1) \cdot (1-r_4) \cdot (1-r_5) \cdot (1-r_6)$$
$$r_5 \cdot (1-r_1) \cdot (1-r_5) \cdot (1-r_6)$$

Taking $r_0 = 0.3055479560$, $r_1 = 0.2499747372$, $r_2 = 0.2063465756$, $r_3 = 0.1924531372$, $r_4 = 0.1818805124$, $r_5 = 0.1958294533$, $r_6 = 0.1602118920$, this is achieved for $x \leq 0.08115$.

2.6.2 Sharper Bound: $x_c \geq 0.08636$

To apply Theorem 18 we need to also consider paths of length 2. To do this we introduce a set of 6 additional variables $r_{1,3}, r_{2,1}, r_{2,4}, r_{3,5}, r_{5,1}, r_{6,1}$ (while, a priori, there are 6^2 "types" of paths of length 2, many of them are infeasible, while for others the type of the first arc implies the type of the second). Specifically, $r_{1,3}$ corresponds to a path first heading east and then heading northwest, $r_{2,1}$ corresponds to a path first heading northeast and then heading east, etc. The resulting 13 inequalities are satisfied for $x \leq 0.08636$ and $r_0 = 0.3939972440$, $r_1 = 0.2956228200$, $r_2 = 0.2271540263$, $r_3 = 0.2187337137$, $r_4 = 0.2144822763$, $r_5 = 0.2060776445$, $r_6 = 0.1736041642$, $r_{1,3} = 0.1820809928$, $r_{2,1} = 0.2347015656$, $r_{2,4} = 0.1772472600$, $r_{3,5} = 0.1675677715$, $r_{5,1} = 0.1868706968$, $r_{6,1} = 0.2417955235$.

3 Relating the Independent Set Polynomial to Walk Trees

3.1 Main Recurrence, Occupation Ratios, and Trees

For $i \in [n]$ and $S \subseteq [n] \setminus \{i\}$, given input $\boldsymbol{x}$, we define

$$Z(\boldsymbol{x}; i \mid S) := \frac{Z(\boldsymbol{x}; S \cup \{i\})}{Z(\boldsymbol{x}; S)} = Z(i \mid S) \ .$$

Trivially, $Z = Z([n]) = \prod_{i \in [n]} Z(i \mid [i-1])$, since $Z(\emptyset) = 1$. To estimate $Z(i \mid S)$ observe that the contribution to $Z(S \cup \{i\})$ of the sets including vertex i equals x_i times the contribution of the sets not including $\Gamma^+(i)$. Therefore,

$$Z(S \cup \{i\}) = Z(S) + x_i Z(S \setminus \Gamma_i) \ . \tag{18}$$

With the above in mind, let $j_1 \geq \ldots \geq j_d$ be the descending ordering of $\Gamma_i \cap S$, and for $\ell \in [d]$ write $S_\ell = S \setminus \{j_1, \ldots, j_\ell\}$. Dividing (18) by $Z(S)$ and writing the ratio $Z(S \setminus \Gamma_i)/Z(S)$ in telescopic form yields

$$Z(i \mid S) = 1 + x_i \frac{1}{\frac{Z(S)}{Z(S \setminus \Gamma_i)}} = 1 + x_i \frac{1}{\prod_{\ell=1}^{d} \frac{Z(S \setminus \{j_1, \ldots, j_{\ell-1}\})}{Z(S \setminus \{j_1, \ldots, j_\ell\})}} = 1 + x_i \prod_{\ell=1}^{d} \frac{1}{Z(j_\ell \mid S_\ell)} \ . \tag{19}$$

It is convenient to introduce the quantity $\mathrm{ratio}_G(\boldsymbol{x}; (i, S)) := Z(i \mid S) - 1 = \mathrm{ratio}(i, S)$ and rewrite (19) as

$$\mathrm{ratio}(i, S) = x_i \prod_{\ell=1}^{d} \frac{1}{1 + \mathrm{ratio}(j_\ell, S_\ell)} \ . \tag{20}$$

Thus,

$$Z = Z([n]) = \prod_{i \in [n]} Z(i \mid [i-1]) = \prod_{i \in [n]} (1 + \mathrm{ratio}(i, [i-1])) \ . \tag{21}$$

We can now characterize the set $\mathcal{S}(G)$ as follows.

▶ **Lemma 19.** *The following are equivalent:*
1. *For every* $S \subseteq [n]$, $Z(-\boldsymbol{p}; S) > 0$.
2. *For every* $i \in [n]$, *and* $S \subseteq [n] \setminus \{i\}$, $\mathrm{ratio}(-\boldsymbol{p}; (i, S)) > -1$.
3. *For every* $i \in [n]$, *and* $S \subseteq [i-1]$, $\mathrm{ratio}(-\boldsymbol{p}; (i, S)) > -1$.

Proof.
($1 \implies 2$) If $Z(S), Z(S \cup \{i\}) > 0$, then $1 + \mathrm{ratio}(i, S) = Z(S \cup \{i\})/Z(S) > 0$.
($2 \implies 3$) Trivial.
($3 \implies 1$) For any $S \subseteq [n]$ and $j \in S$, write $S_j = \{k \in S : k < j\}$. By telescoping, $Z(S) = \prod_{j \in S} Z(j|S_j) = \prod_{j \in S}(1 + \mathrm{ratio}(j, S_j))$. Since $S_j \subseteq [i-1]$, the last product is positive. ◀

Say that $S, T \subseteq [n]$ are *separate* if they are disjoint and no edge has one endpoint in each. Clearly, if S, T are separate, then $Z(S \cup T) = Z(S)Z(T)$. Moreover, if $T \subseteq [n]$ is separate from $S \cup \{i\}$, then

$$\begin{aligned} \mathrm{ratio}(i, S \cup T) &= x_i \frac{Z((S \cup T) \setminus \Gamma_i)}{Z(S \cup T)} \\ &= x_i \frac{Z((S \setminus \Gamma_i) \cup T)}{Z(S \cup T)} \\ &= x_i \frac{Z(S \setminus \Gamma_i) Z(T)}{Z(S)Z(T)} = \mathrm{ratio}(i, S) \ . \end{aligned} \tag{22}$$

▶ **Definition 20.** *For a vertex v of a rooted tree T, we use $\widehat{\mathrm{ratio}}_T(v)$ to denote the quantity $\mathrm{ratio}_T(v, T(v))$, where $T(v)$ is the set of vertices other than v in the subtree rooted at v.*

Using (22) we observe that for a rooted tree T, recurrence (20) can be rewritten as

$$\widehat{\mathrm{ratio}}_T(v) = x_v \prod_{\ell=1}^{d} \frac{1}{1 + \widehat{\mathrm{ratio}}_T(v_\ell)} \ , \tag{23}$$

where $\{v_1, \ldots, v_d\}$ are the children of v in T.

3.2 Relating Arbitrary Graphs to Walk-Trees

Let $w = (v_0, v_1, \ldots, v_\ell)$ be an arbitrary walk of length ℓ.

▶ **Definition 21.** *w is* self-avoiding *if its vertices are* distinct.

▶ **Definition 22.** *w is* descending *if $v_k < v_{k-1}$ for all $k \in [\ell]$.*

Recall that, per Definition 16, for a walk $w = (v_0, v_1, \ldots, v_\ell)$, we let $\mathcal{F}(v_0) = \emptyset$, while for $k \in [\ell]$ we let $\mathcal{F}(v_0, \ldots, v_k) = \mathcal{F}(v_0, \ldots, v_{k-1}) \cup \{v_{k-1}\} \cup \{u \in \Gamma_{v_{k-1}} : u \geq v_k\}$.

▶ **Definition 23.** *$w = (v_0, v_1, \ldots, v_\ell)$ is* self-bounding *if $v_{k+1} \notin \mathcal{F}(v_0, \ldots, v_k)$ for all $k \in [\ell]$.*

▶ Remark 24. Self-bounding walks were defined in [17] as "truncated self-avoiding walks." The idea is that the next vertex in a self-bounding walk is subject to the additional requirement, relative to a self-avoiding walk, that it can also not be connected to certain neighbors of previously visited vertices. While a descending walk is self-bounding, the converse need not hold. For instance, in $G = ([4], \{\{1, 2\}, \{2, 3\}, \{3, 4\}, \{4, 1\}\})$, the walk $(4, 1, 2)$ is self-bounding but not descending.

For $S \subseteq [n]$, we write G_S for the subgraph of G induced by S.

▶ **Definition 25.** *Let $\mathcal{W}$ be a set of walks on G all starting at i, such that if $w \in \mathcal{W}$, then the same is true for every prefix of w. The* walk-tree *corresponding to the set of walks $\mathcal{W}$ has as its root the walk (i) of length 0, while the children of each vertex (walk) are its extensions by one step. The* activity *of vertex $(i, v_1, \ldots, v_\ell)$ of the walk-tree is x_{v_ℓ}.*

We use $\mathcal{L}_i := \mathcal{L}_i(G)$ to denote the walk-tree of self-bounding walks on $G_{[i]}$ starting at i.

The following theorem reduces the computation of ratios of an arbitrary graph G, to that of the tree ratios of $\mathcal{L}_i(G)$.

▶ **Theorem 26.** *For every vertex $i \in [n]$ and every walk $w = (v_0, v_1, \ldots, v_\ell)$ in $\mathcal{L}_i$,*

$$\widehat{\text{ratio}}_{\mathcal{L}_i}(w) = \text{ratio}_G\left(v_\ell, [i-1] \setminus \mathcal{F}(v_0, \ldots, v_\ell)\right) \quad . \tag{24}$$

In particular, $\widehat{\text{ratio}}_{\mathcal{L}_i}((i)) = \text{ratio}_G(i, [i-1])$.

Proof. We proceed by induction on the size of the subtree rooted at w.

If w is a leaf in $\mathcal{L}_i$ then, trivially, $\text{ratio}_{\mathcal{L}_i}(w) = x_{v_\ell}$ and $\mathcal{F}(v_0, \ldots, v_\ell) \supseteq \Gamma_{v_\ell}$, for otherwise w could be extended. Thus, $[i-1] \setminus \mathcal{F}(v_0, \ldots, v_\ell)$ is separate from v_ℓ, which per (22) implies that $\text{ratio}_G(v_\ell, [i-1] \setminus \mathcal{F}(v_0, \ldots, v_\ell)) = \text{ratio}_G(v_\ell, \emptyset) = x_{v_\ell}$.

If w is not a leaf in $\mathcal{L}_i$, assume the theorem holds for its descendants. Let $\{j_1, \ldots, j_d\} = \Gamma_{v_\ell} \cap ([i-1] \setminus \mathcal{F}(v_0, \ldots, v_\ell))$, with $j_1 \geq \ldots \geq j_d$, and for $t \in [d]$ write $w_t = (v_0, v_1, \ldots, v_\ell, j_t)$. The first equality below follows from (23), the second from the inductive hypothesis, the third from the definition of $\mathcal{F}$, and the last from (20):

$$\widehat{\text{ratio}}_{\mathcal{L}_i}(w) = x_{v_\ell} \prod_{t=1}^{d} \frac{1}{1 + \widehat{\text{ratio}}_{\mathcal{L}_i}(w_t)} \tag{25}$$

$$= x_{v_\ell} \prod_{t=1}^{d} \frac{1}{1 + \text{ratio}_G\left(j_t, [i-1] \setminus \mathcal{F}\left(v_0, \ldots, v_\ell, j_t\right)\right)} \tag{26}$$

$$= x_{v_\ell} \prod_{t=1}^{d} \frac{1}{1 + \text{ratio}_G\left(j_t, ([i-1] \setminus \mathcal{F}\left(v_0, \ldots, v_\ell\right)) \setminus \{j_1, \ldots, j_t\}\right)} \tag{27}$$

$$= \text{ratio}_G\left(v_\ell, [i-1] \setminus \mathcal{F}\left(v_0, \ldots, v_\ell\right)\right) \quad . \tag{28}$$

◀

3.3 Tree Monotonicity

▶ **Definition 27.** *Let T be a tree with root r. The set of* prefixes *of T comprises T itself, and every tree with root r that can be derived by removing a leaf from a prefix of T.*

▶ **Lemma 28.** *Let T be a tree with root r and assume that $\boldsymbol{p}$ is such that $\widehat{\text{ratio}}_T(-\boldsymbol{p}; v) > -1$ for every vertex $v \neq r$ of T. Then the function $f : \boldsymbol{x} \mapsto \widehat{\text{ratio}}_T(-\boldsymbol{x}; r)$ is smooth and strictly decreasing in each coordinate inside $P = \{(x_1, \ldots, x_n) : 0 \leq x_i \leq p_i\}$. In particular, if T' is a prefix of T, then $\widehat{\text{ratio}}_T(-\boldsymbol{p}; r) \leq \widehat{\text{ratio}}_{T'}(-\boldsymbol{p}; r)$.*

Proof. We use induction on the size of T. If T consists of just $\{r\}$, then $\widehat{\text{ratio}}_T(-\boldsymbol{x}; r) = -x_r$, satisfying the claim trivially. Let now T be a tree of size n, and assume that the lemma holds for every tree of size strictly less than n. If $\Gamma_i = \{j_1, \ldots, j_d\}$, then per (23),

$$\widehat{\text{ratio}}_T(-\boldsymbol{x}; r) = -x_r \prod_{\ell=1}^{d} \frac{1}{1 + \widehat{\text{ratio}}_T(-\boldsymbol{x}; j_\ell)} \quad . \tag{29}$$

Since each subtree rooted at j_ℓ has size strictly less than n, the inductive hypothesis implies that $\widehat{\text{ratio}}_T(-\boldsymbol{x}; j_\ell)$ is strictly decreasing inside P. Therefore, the lemma hypothesis that $\widehat{\text{ratio}}_T(-\boldsymbol{p}; j_\ell) > -1$ implies that $\widehat{\text{ratio}}_T(-\boldsymbol{x}; j_\ell) > -1$. Since the function $1/(1+x)$ is smooth and strictly decreasing for $x > -1$, the claim follows by the smoothness and monotonicity of the d factors in (29) implied by the inductive hypothesis.

To see the claim regarding prefixes of T, observe that $\widehat{\text{ratio}}_{T'}(-\boldsymbol{p}; r) = \widehat{\text{ratio}}_T(-\boldsymbol{p}'; r)$, where $\boldsymbol{p}'$ is derived by setting to 0 all coordinates of $\boldsymbol{p}$ corresponding to vertices not in T'. ◀

▶ **Theorem 29.** *$\boldsymbol{p} \in \mathcal{S}(G)$ iff $\widehat{\text{ratio}}_{\mathcal{L}_i}(-\boldsymbol{p}; w) > -1$, for all $i \in [n]$ and $w \in \mathcal{L}_i$.*

Proof. If $\boldsymbol{p} \in \mathcal{S}(G)$, then, by Lemma 19, $\text{ratio}_G(i, S) > -1$, for every $i \in [n]$ and $S \subseteq [n] \setminus \{i\}$. Thus, per Theorem 26, $\widehat{\text{ratio}}_{\mathcal{L}_i}(-\boldsymbol{p}; w) = \text{ratio}_G(v_\ell, [i-1] \setminus \mathcal{F}(v_0, \ldots, v_\ell)) > -1$.

For the converse, we will show that if $\widehat{\text{ratio}}_{\mathcal{L}_i}(-\boldsymbol{p}; w) > -1$ for all $i \in [n]$ and $w \in \mathcal{L}_i$, then $\text{ratio}(i, S) > -1$ for every $i \in [n]$ and $S \subseteq [i-1]$, which, by Lemma 19, implies $\boldsymbol{p} \in \mathcal{S}(G)$. Let $i \in [n]$ and $S \subseteq [i-1]$ be arbitrary, write $S^+ := S \cup \{i\}$, and let $\widetilde{\mathcal{L}}_i$ be the prefix of $\mathcal{L}_i$ obtained by deleting all walks intersecting the complement of S^+. It is easy to check that $\widetilde{\mathcal{L}}_i$ coincides with the tree of self-bounding walks starting at i on the subgraph of $G_{[i]}$ induced by S^+, i.e., $\widetilde{\mathcal{L}}_i(G) = \mathcal{L}_i(G_{S^+})$. Thus, Theorem 26 gives the second equality below, while the monotonicity of tree prefixes, per Lemma 28, gives the first inequality:

$$\text{ratio}_G(-\boldsymbol{p}; (i, S)) = \text{ratio}_{G_{S^+}}(-\boldsymbol{p}; (i, S)) = \widehat{\text{ratio}}_{\widetilde{\mathcal{L}}_i}(-\boldsymbol{p}; (i)) \geq \widehat{\text{ratio}}_{\mathcal{L}_i}(-\boldsymbol{p}; (i)) > -1 \ . \quad ◀$$

4 Proofs of Results

4.1 Upper Bound (Theorem 9)

Let $\mathcal{D}_i := \mathcal{D}_i(G)$ denote the tree of descending walks on G starting at i. Due to its highly recursive structure, if two vertices in $\mathcal{D}_i$ correspond to walks that end on the same vertex, then their ratios are equal. As a result, the different root ratios satisfy the following simple system of equations.

▶ **Theorem 30.** *Given $\boldsymbol{x} \in \mathbb{C}^n$, for $i = 1, 2, \ldots, n$ let*

$$r_i = x_i \prod_{j \in \overleftarrow{\Gamma}_i} \frac{1}{1 + r_j} \ . \tag{30}$$

Then, $\widehat{\text{ratio}}_{\mathcal{D}_i}(\boldsymbol{x}; (i)) = r_i$, for every $i \in [n]$.

Proof. We use induction on i. For $i = 1$, trivially, $\widehat{\text{ratio}}_{\mathcal{D}_1}(\boldsymbol{x}; (1)) = x_1 = r_1$. Assume now that (30) holds for all $i < k$. Clearly, the root walk (k) can only be extended by taking a step to a neighbor smaller than k. If $\{j_1, \ldots, j_d\} = \overleftarrow{\Gamma}_k$, then (23) yields (31). For the first equality in (32), note that appending k as a prefix to every vertex of $\mathcal{D}_{j_\ell}$ yields the subtree of $\mathcal{D}_k$ rooted at (k, j_ℓ), while the inductive hypothesis yields the second equality in (32).

$$\widehat{\text{ratio}}_{\mathcal{D}_k}(\boldsymbol{x}; (k)) = x_k \prod_{\ell=1}^{d} \frac{1}{1 + \widehat{\text{ratio}}_{\mathcal{D}_k}(\boldsymbol{x}; (k, j_\ell))} \tag{31}$$

$$= x_k \prod_{\ell=1}^{d} \frac{1}{1 + \widehat{\text{ratio}}_{\mathcal{D}_{j_\ell}}(\boldsymbol{x}; (j_\ell))} = x_i \prod_{j \in \overleftarrow{\Gamma}_i} \frac{1}{1 + r_j} = r_k \ . \tag{32}$$

◀

Proof of Theorem 9. Without loss of generality, we assume that π is the identity. Equation (21) yields (33), while (34) follows from Theorem 26. Recalling that descending walks are self-bounding shows that $\mathcal{D}_i$ is a prefix of $\mathcal{L}_i$ and, thus, per Lemma 28, $\widehat{\text{ratio}}_{\mathcal{D}_i}(-\boldsymbol{p}; (i)) \geq \widehat{\text{ratio}}_{\mathcal{L}_i}(-\boldsymbol{p}; (i))$, yielding (35). Finally, our hypothesis is equivalent to $-r_i$ satisfying (30) for $\boldsymbol{x} = -\boldsymbol{p}$ so that Theorem 30, implies $\widehat{\text{ratio}}_{\mathcal{D}_i}(-\boldsymbol{p}; (i)) = -r_i$ and, thus, (36).

$$Z(-\boldsymbol{p}; S) = \prod_{i \in [n]} (1 + \text{ratio}_G(-\boldsymbol{p}; (i, [i-1]))) \tag{33}$$
$$= \prod_{i \in [n]} \left(1 + \widehat{\text{ratio}}_{\mathcal{L}_i}(-\boldsymbol{p}; (i))\right) \tag{34}$$
$$\leq \prod_{i \in [n]} \left(1 + \widehat{\text{ratio}}_{\mathcal{D}_i}(-\boldsymbol{p}; (i))\right) \tag{35}$$
$$= (1 - r_i) \ . \tag{36}$$

◀

4.2 Chordal Graphs (Theorem 12)

We claim that a graph on $[n]$ is chordally presented iff its set of descending walks equals its set of self-bounding walks. Given this claim, Theorem 12 follows from Theorem 30. Since descending walks are self-bounding, the following suffices to prove our claim.

▶ **Theorem 31.** *G is not chordally presented iff there is a vertex i and a self-bounding walk on $G_{[i]}$ starting at i that is not descending.*

Proof. Let $(i =: v_0, v_1, \dots, v_\ell)$ be a self-bounding walk on $G_{[i]}$ that is not descending and let $2 \leq k \leq \ell$ be the minimum index such that $v_{k-1} < v_k$. The minimality of k implies $v_{k-1} < v_{k-2}$ and, hence, that $v_k, v_{k-2} \in \overrightarrow{\Gamma}_{v_{k-1}}$. Since the walk is self-bounding, $v_k \notin \Gamma_{v_{k-2}}$, i.e., there is no edge between v_{k-2} and v_k, implying that G is not chordally presented.

If G is not chordally presented, there must be vertices $a < b < c$ such that a is connected to b and c, but b is not connected to c. Clearly, the walk (c, a, b) on $G_{[c]}$ is self-bounding but not descending. ◀

4.3 Proof of Theorem 7 given Theorem 14

Proof. Given $\{r'_i\}_{i \in [n]}$, let $r_i = r'_i$ and $r_{i,j} = r'_i \frac{1-r'_j}{1-r'_i r'_j}$. We show that if (4) is satisfied, then (7) and (8) are satisfied. Indeed,

$$r_i \prod_{j \in \Gamma_i} (1 - r_{j,i}) = r'_i \prod_{j \in \Gamma_i} \left(1 - r'_j \frac{1 - r'_i}{1 - r'_j r'_i}\right) = r'_i \prod_{j \in \Gamma_i} \left(\frac{1 - r'_j}{1 - r'_j r'_i}\right) \geq p_i \ ,$$

and

$$r_{i,j} \prod_{k \in \Gamma_i \setminus \{j\}} (1 - r_{k,i}) = r'_i \frac{1 - r'_j}{1 - r'_i r'_j} \prod_{k \in \Gamma_i \setminus \{j\}} \left(1 - r'_k \frac{1 - r'_i}{1 - r'_k r'_i}\right) = r'_i \prod_{j \in \Gamma_i} \left(\frac{1 - r'_j}{1 - r'_j r'_i}\right) \geq p_i.$$

◀

4.4 Proof of Theorem 18

Proof. We claim that (15)–(17) imply $\text{ratio}(-\boldsymbol{p}; (i, S)) \geq -r_i$ for all $i \in [n]$ and $S \subseteq [n] \setminus \{i\}$. This suffices since $Z([n]) = \prod_{i=1}^n Z(i|[i-1]) = \prod_{i=1}^n (1 + \text{ratio}(i, [i-1])) \geq \prod_{i=1}^n (1 - r_i)$.

To prove the claim we prove that if (15)–(17) hold, then (a),(b),(c) below hold (our claim is equivalent to (a); we only prove (b), (c) as aids for proving (a)):

(a) $\text{ratio}(-\boldsymbol{p}; (i, S)) \geq -r_i$, for every (empty) path (i) and every $S \subseteq [n] \setminus \{i\}$.

(b) $\text{ratio}(-\boldsymbol{p}; (j, S)) \geq -r_{i,j}$, for every path (i, j) and every $S \subseteq [n] \setminus \mathcal{N}(i, j)$.

(c) $\text{ratio}(-\boldsymbol{p}; (k, S)) \geq -r_{i,j,k}$, for every path (i, j, k) such that $\mathcal{N}(i, j, k) \neq \mathcal{N}(j, k)$ and every $S \subseteq [n] \setminus \mathcal{N}(i, j, k)$.

To prove (a),(b),(c) we proceed by induction on $|S|$. For $S = \emptyset$, we see that (15)–(17) imply $-p_i \geq \max\{-r_{k,j,i}, -r_{j,i}, -r_i\}$, for any $i, j, k \in [n]$, while $\text{ratio}(-\boldsymbol{p}; (i, S)) = -p_i$.

For $S \neq \emptyset$, assume that (a),(b),(c) hold for all sets of size strictly less than $|S|$.

(a) For any path (i) and any set $S \subseteq [n] \setminus \{i\}$, equation (20) implies the first equality below, while the inductive hypothesis yields the first inequality (since $\mathcal{N}(i, j)$ is non-empty):

$$\begin{aligned}
\text{ratio}(i, S) &= -p_i \prod_{j \in S \cap \Gamma_i} \frac{1}{1 + \text{ratio}(j, S \setminus \mathcal{N}(i, j))} \\
&\geq -p_i \prod_{j \in S \cap \Gamma_i} \frac{1}{1 - r_{i,j}} \\
&\geq -p_i \prod_{j \in \Gamma_i} \frac{1}{1 - r_{i,j}} \quad .
\end{aligned}$$

Assumption (15) concludes the argument.

(b) For any path (i, j) and any set $S \subseteq [n] \setminus \mathcal{N}(i, j)$, equation (20) implies the first equality below, the second equality holds since S is devoid of vertices from $\mathcal{N}(i, j)$, while the third equality follows easily from the definition of $\mathcal{N}$:

$$\begin{aligned}
\text{ratio}(j, S) &= -p_j \prod_{k \in S \cap \Gamma_j} \frac{1}{1 + \text{ratio}(k, S \setminus \mathcal{N}(j, k))} \\
&= -p_j \prod_{k \in S \cap \Gamma_j} \frac{1}{1 + \text{ratio}(k, S \setminus (\mathcal{N}(i, j) \cup \mathcal{N}(j, k)))} \\
&= -p_j \prod_{k \in S \cap \Gamma_j} \frac{1}{1 + \text{ratio}(k, S \setminus \mathcal{N}(i, j, k))} \qquad (37)
\end{aligned}$$

Decomposing the product in (37) into two groups of factors yields (38) and invoking the inductive hypothesis yields (39):

$$\prod_{\substack{k \in S \cap \Gamma_j \\ \mathcal{N}(i,j,k) = \mathcal{N}(j,k)}} \left(\frac{1}{1 + \text{ratio}(k, S \setminus \mathcal{N}(j, k))} \right) \prod_{\substack{k \in S \cap \Gamma_j \\ \mathcal{N}(i,j,k) \neq \mathcal{N}(j,k)}} \left(\frac{1}{1 + \text{ratio}(k, S \setminus \mathcal{N}(i, j, k))} \right) \qquad (38)$$

$$\leq \prod_{\substack{k \in S \cap \Gamma_j \\ \mathcal{N}(i,j,k) = \mathcal{N}(j,k)}} \left(\frac{1}{1 - r_{j,k}} \right) \prod_{\substack{k \in S \cap \Gamma_j \\ \mathcal{N}(i,j,k) \neq \mathcal{N}(j,k)}} \left(\frac{1}{1 - r_{i,j,k}} \right) \qquad (39)$$

$$\leq \prod_{\substack{k \in \Gamma_j \setminus \mathcal{N}(i,j) \\ \mathcal{N}(i,j,k) = \mathcal{N}(j,k)}} \left(\frac{1}{1 - r_{j,k}} \right) \prod_{\substack{k \in \Gamma_j \setminus \mathcal{N}(i,j) \\ \mathcal{N}(i,j,k) \neq \mathcal{N}(j,k)}} \left(\frac{1}{1 - r_{i,j,k}} \right) \quad .$$

Assumption (16) concludes the argument.

(c) For any path (i,j,k) such that $\mathcal{N}(i,j,k) \neq \mathcal{N}(j,k)$ and any set $S \subseteq [n] \setminus \mathcal{N}(i,j,k)$, equation (20) implies the first equality below, the second equality holds since S is devoid of vertices from $\mathcal{N}(j,k)$, while the third equality follows easily from the definition of $\mathcal{N}$:

$$\begin{aligned}\mathrm{ratio}(k,S) &= -p_k \prod_{\ell \in S \cap \Gamma_k} \frac{1}{1+\mathrm{ratio}(\ell, S \setminus \mathcal{N}(k,\ell))} \\ &= -p_k \prod_{\ell \in S \cap \Gamma_k} \frac{1}{1+\mathrm{ratio}(\ell, S \setminus (\mathcal{N}(j,k) \cup \mathcal{N}(k,\ell)))} \\ &= -p_k \prod_{\ell \in S \cap \Gamma_k} \frac{1}{1+\mathrm{ratio}(\ell, S \setminus \mathcal{N}(j,k,\ell))} \ . \end{aligned} \tag{40}$$

Decomposing the product in (40) into two groups of factors yields (41) and invoking the inductive hypothesis yields (42):

$$\prod_{\substack{\ell \in S \cap \Gamma_k \\ \mathcal{N}(j,k,\ell) = \mathcal{N}(k,\ell)}} \left(\frac{1}{1+\mathrm{ratio}(\ell, S \setminus \mathcal{N}(k,\ell))} \right) \prod_{\substack{\ell \in S \cap \Gamma_j \\ \mathcal{N}(j,k,\ell) \neq \mathcal{N}(k,\ell)}} \left(\frac{1}{1+\mathrm{ratio}(\ell, S \setminus \mathcal{N}(j,k,\ell))} \right) \tag{41}$$

$$\leq \prod_{\substack{\ell \in S \cap \Gamma_k \\ \mathcal{N}(j,k,\ell) = \mathcal{N}(k,\ell)}} \left(\frac{1}{1 - r_{k,\ell}} \right) \prod_{\substack{\ell \in S \cap \Gamma_k \\ \mathcal{N}(j,k,\ell) \neq \mathcal{N}(k,\ell)}} \left(\frac{1}{1 - r_{j,k,\ell}} \right) \tag{42}$$

$$\leq \prod_{\substack{\ell \in \Gamma_k \setminus \mathcal{N}(i,j,k) \\ \mathcal{N}(j,k,\ell) = \mathcal{N}(k,\ell)}} \left(\frac{1}{1 - r_{k,\ell}} \right) \prod_{\substack{\ell \in \Gamma_k \setminus \mathcal{N}(i,j,k) \\ \mathcal{N}(j,k,\ell) \neq \mathcal{N}(k,\ell)}} \left(\frac{1}{1 - r_{j,k,\ell}} \right) \ .$$

Assumption (17) concludes the argument. ◀

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