Report of Dagstuhl Seminar 16071

Pattern Avoidance and Genome Sorting

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— Abstract

This report documents the program and the outcomes of Dagstuhl Seminar 16071 "Pattern Avoidance and Genome Sorting".

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Edited in cooperation with Miklós Bóna

1 Executive Summary

Miklós Bóna

The seminar took place from February 14, 2016, to February 19, 2016. It had 36 participants, who were researchers in theoretical computer science, combinatorics, and molecular biology. It was a geographically diverse group, with participants coming from the US, Canada, Brazil, Germany, Iceland, the United Kingdom, Sweden, France, Slovakia, Hungary and New Zealand. The seminar featured 18 talks, three of which were hourlong talks, and an open problem session.

Numerous collaborative research efforts have been started. Here is a sampling.

Megan Martinez and Manda Riehl worked on a bijection between LP matchings (one of the RNA matchings described in Vincent Vatter's talk) and Klazar's nesting equivalent matchings. They studied a paper by Klazar and Aziza Jefferson's dissertation and made progress on the bijection.

István Miklós, Péter Erdős and Miklós Bóna worked on proving a log-convexity conjecture related to ordered degree sequences of bipartite graphs.

Brona Brejova and Manda Riehl discussed two potential future projects related to gene and species tree reconciliation. The most probable starting point is a project involving gene and species trees where a gene is allowed to duplicate a string inside itself. This situation was not allowed in previous models, however it seems that as long as the specific breakpoints are not reused from this insertion, a modification of the previous algorithms could still be effective.

Jay Pantone, David Bevan and Miklós Bóna collaborated on asymptotic enumeration of a balanced urns and balls model that was seen to be a step towards finding a better upper bound for a pattern avoidance enumeration problem.

We have all the reasons to believe that this, and many other joint research efforts that started during this seminar will lead to new results that would not have been possible without the seminar. Therefore, we strongly believe that the seminar was a success that we would like to repeat at some point in the future.

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3 Overview of Talks

3.1 Decomposition trees of permutations, and how to use them for a (realistic?) study of perfect sorting by reversals

Mathilde Bouvel (Universität Zürich, CH)

Joint work of Mathilde Bouvel, Cedric Chauve, Marni Mishna, Cyril Nicaud, Carine Pivoteau, and Dominique Rossin

Main reference M. Bouvel, M. Mishna, C. Nicaud, "Some simple varieties of trees arising in permutation analysis", in Proc. of the 25th Int'l Conf. on Formal Power Series and Algebraic Combinatorics (FPSAC 2013), DMTCS proceedings, 2013.

URL http://www.dmtcs.org/dmtcs-ojs/index.php/proceedings/issue/view/130

 ${\tt URL \ http://user.math.uzh.ch/bouvel/presentations/Poster2013_BMN.pdf}$

I will present the genome rearrangement problem of perfect sorting by reversals, and show its algorithmic solution by Bérard-Bergeron-Chauve-Paul. It uses the strong interval trees of permutations (whose definition will be recalled in the talk). Those trees are also known as (substitution) decomposition trees of permutations. I will present two results and a research project related to those trees.

First, I will show that the algorithm of Bérard-Bergeron-Chauve-Paul is polynomial on average (and with probability 1 as the size of the input goes to infinity). I will also describe average properties of commuting scenarios (a.k.a. separable permutations) for perfect sorting by reversals. These results are obtained using the tools of analytic combinatorics developed by Flajolet-Sedgewick.

Second, I will generalize these average properties (to some extent) to super-classes of the separable permutations. This demonstrates a phenomenon of convergence of a sequence of families of trees to the class of all permutations, whose analytic nature is essentially different. We only have a partial explanation of this phenomenon.

Finally, I will go back to the biological motivation, showing that all these models of trees do not represent well the strong interval trees obtained from the biological data. I will conclude by proposing a possibly better model, whose study is yet to be done.

3.2 Isometric Gene Tree Reconciliation

Brona Brejova (Comenius University in Bratislava, SK)

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The infinite sites model, introduced by Jian Ma et al (PNAS 2008), formalizes the problem of recovering the evolutionary history of a set of related genomes allowing a large set of evolutionary operations including insertions, deletions, duplications, and rearrangements. One of the steps of their polynomial-time algorithm reconciles a gene tree with a species tree under the assumption that both trees have exact branch lengths known. This assumption simplifies the problem compared to the typical reconciliation scenario without branch lengths. We show several mistakes in the original algorithm and provide a corrected and simplified version. We also discuss related open problems.

3.3 The SCJ small parsimony problem for weighted gene adjacencies

Cedric Chauve (Simon Fraser University – Burnaby, CA)

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 Joint work of Ashok Rajaraman, Yann Ponty, Cedric Chauve

 Main reference A. Rajaraman, C. Chauve, Y. Ponty, "Assessing the Robustness of Parsimonious Predictions for
 Gene Neighborhoods from Reconciled Phylogenies: Supplementary Material", Bioinformatics
 Research and Applications, LNCS, Vol. 9096, pp. 260–271, Springer, 2015.

 URL http://dx.doi.org/10.1007/978-3-319-19048-8_22

Reconstructing ancestral gene orders in a given phylogeny is a classical problem in comparative genomics. Most existing methods compare conserved features in extant genomes in the phylogeny to define potential ancestral gene adjacencies, and either try to reconstruct all ancestral genomes under a global evolutionary parsimony criterion, or, focusing on a single ancestral genome, use a scaffolding approach to select a subset of ancestral gene adjacencies, generally aiming at reducing the fragmentation of the reconstructed ancestral genome. We describe an exact algorithm for the small parsimony problem that combines both approaches. We consider that gene adjacencies at internal nodes of the species phylogeny are weighted, and we introduce an objective function defined as a convex combination of these weights and the evolutionary cost under the Single-Cut-or-Join (SCJ) model. The weights of ancestral gene adjacencies can e.g. be obtained through the recent availability of ancient DNA sequencing data, which provide a direct hint at the genome structure of the considered ancestor, or through probabilistic analysis of gene adjacencies evolution. The algorithm we propose is Fixed-Parameter Tractable (FPT) based on the dynamic programming algorithm by (Sankoff and Rousseau, 1975) and allows to sample co-optimal solutions.

3.4 Method of moments estimates for reversal and block transposition distances using symmetric group models

Niklas Eriksen (University of Örebro, SE)

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 Joint work of Niklas Eriksen, Axel Hultman
 Main reference N. Eriksen, A. Hultman, "Expected reflection distance in G(r,1,n) after a fixed number of reflections", Annals of Combinatorics, 9(1):21–33, Springer, 2005.
 URL http://dx.doi.org/10.1007/s00026-005-0238-y

The gene order of species change over time, and can hence be used to infer relationships between species. By estimating the number of reversals or block transpositions that separate two species, we get an idea of the time since speciation. Eriksen and Hultman introduced a permutation model with similar properties to the reversal model but much more tractable. In this model, method of moments estimates could be computed, corresponding to the reversal distance in a pure reversal model. We extend their results to obtain several estimates of the number of reversal and block transpositions that separate two species. We also give a method for estimating the proportion on reversals, which is a very important parameter.

3.5 Gene orders, median of permutations and related combinatorial problems

Sylvie Hamel (University of Montréal, CA)

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 Joint work of Sylvie Hamel and Robin Milosz

 Main reference
 R. Milosz, S. Hamel, "Medians of Permutations: building constraints", Algorithms and Discrete Applied Mathematics, LNCS, Vol. 9602, pp. 264–276, Springer, 2016.
 URL http://dx.doi.org/10.1007/978-3-319-29221-2_23

Our aim is to discuss the general problem of finding a consensus ranking, given a set of different rankings of a set of objects. Here, one assumes that a set of different rankings are proposed for a given set of strictly ordered elements, and one is looking for a ranking that is in closest agreement to all of these. Thus, the problem becomes that of finding the median of a set of permutations under a distance d. In part this is motivated by the classical gene order problem of comparative genomics, where the difference in the order of appearance of genes in the genome of different species is used to evaluate the evolutionary distances between them.

We give close attention to this median problem for the "Kendall-tau" distance, which corresponds to counting the number of order disagreements between pairs of elements of two permutations. The problem has been shown to be NP-complete for sets of m permutations, where m > 3, and the complexity is still unknown for m = 3. From an algorithmic point of view, we present a deterministic heuristic for this median problem, and derive some theoretical properties of the starting set of permutations that drastically reduce the search space for the medians of this set. In a more combinatoric point of view, we consider the interesting automedian cases (when a set of permutations is equal to the set of its medians), deriving some of its properties under group actions, shuffle operation, etc. Finally, we generalize this problem to the problem of "aggregating ranking with ties", with an application to the bioinformatic context of calculating such medians for biological data related to certain diseases.

3.6 Sorting with Forbidden Intermediates

Anthony Labarre (University Paris-Est – Marne-la-Vallée, FR)

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Most genome rearrangement problems on permutations can be recast as constrained sorting problems, where the goal is to compute of a shortest sorting sequence of operations for a given permutation under the restriction that the set of allowed operations is fixed beforehand. However, biologists have known for more than a century that some of these mutations at a given point in time can be lethal to a given organism. We revisit those problems by adding a new constraint on the sequences to be computed: they must avoid a given set of forbidden intermediates, which correspond to species that cannot exist because the mutations that would be involved in their creation are lethal. We initiate this study by focusing on the case where the only mutations that can occur are algebraic transpositions, and give a polynomial time algorithm for solving that problem when the permutation to sort is an involution.

3.7 Efficient algorithms for permutation pattern matching

Marie-Louise Lackner (TU Wien, AT)

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 Joint work of Michael Albert, Marie-Louise Lackner, Martin Lackner and Vincent Vatter

 Main reference M. H. Albert, M.-L. Lackner, M. Lackner, V. Vatter, "The complexity of pattern matching for 321-avoiding and skew-merged permutations", arXiv:1510.06051 [math.CO], 2015.

 URL http://arxiv.org/abs/1510.06051v1

Given two permutations τ and π where π , the pattern, is shorter than τ , the Permutation Pattern Matching problem (PPM) asks whether π is contained in τ . In general, this problem is known to be NP-complete, implying that we may not hope for efficient algorithms to solve PPM. Two directions have been pursued so far in order to circumvent this hardness result: First, one can look for special cases in which PPM can be solved efficiently, i.e., in polynomial time. Second, one can try to find a parameter that explains the computational hardness of this problem and confine the combinatorial explosion to this parameter. In this talk, I will give an overview of the algorithms known so far and present one algorithm following the first approach and one taking the second one in more detail.

3.8 Social choice and permutation patterns

Martin Lackner (University of Oxford, GB)

In this talk I will discuss several combinatorial and algorithmic problems from Social Choice and how to they relate to questions about permutation patterns. In particular, some questions about structure in preferences can be answered by translating them to questions about permutation patterns. Also, I will present open problems about permutation patterns that arise from questions in Social Choice.

3.9 Counting and sampling genome rearrangement scenarios: a meeting-point of combinatorics and computer science

István Miklós (Alfréd Rényi Institute of Mathematics – Budapest, HU)

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 Joint work of István Miklós, Heather Smith
 Main reference I. Miklós and H. Smith, "Sampling and counting genome rearrangement scenarios", BMC Bioinformatics, 16(Suppl 14):S6, Springer, 2015.

 URL http://dx.doi.org/10.1186/1471-2105-16-S14-S6

Even for moderate size inputs, there are a tremendous number of optimal rearrangement scenarios, regardless what the model is and which specific question is to be answered. Therefore giving one optimal solution might be misleading and cannot be used for statistical inferring. Statistically well funded methods are necessary to sample uniformly from the solution space and then a small number of samples are sufficient for statistical inferring.

In this talk, we are going to give an overview of the state-of-the-art of sampling and counting rearrangement scenarios. The talk will focus on how combinatorial methods can be used in computational statistics.

3.10 The method of differential approximants

Jay Pantone (Dartmouth College – Hanover, US)

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For decades, the method of differential approximants has been applied to the study of statistical mechanics to estimate the singularity structure of the generating function of a sequence of positive integers, using only a finite number of initial terms of the generating function. While all such approximations are of course only non-rigorous estimates, experience shows these estimates to be remarkably accurate.

Differential approximants can be extremely useful to combinatorialists. We provide several examples of combinatorial sequences for which no generating function is known or conjectured yet the method of differential approximants provides a very accurate approximation of the asymptotic behavior of the sequence. We then describe several extensions to the method that are in progress.

3.11 Parametric Analysis of an SCFG-based model for RNA structure prediction

Svetlana Poznanovikj (Clemson University, US)

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The function of the RNA molecule is often dependent on its structure and so understanding how the RNA nucleotide chain folds onto itself is an important problem. Language-based methods for RNA structure prediction use stochastic context-free grammars (SCFGs). The SCFG developed by Knudsen and Hein is relatively simple and yet has been shown to achieve good accuracy compared to other grammars. We performed an analysis of the probability distribution induced by this grammar and in this talk I'll present some interesting properties that we found.

3.12 Longest increasing subsequences and log concavity

Bruce Sagan (Michigan State University – East Lansing, US), Miklós Bóna (University of Florida – Gainesville, US), and Marie-Louise Lackner (TU Wien, AT)

Let \mathfrak{S}_n be the set of all permutations of $1, 2, \ldots, n$ viewed as sequences. Let $l_{n,k}$ be the number of $\pi \in \mathfrak{S}_n$ having a longest increasing subsequence of length k. This length is closely related to the Ulam distance between permutations which is used to model evolutionary distance in DNA research. William Chen conjectured that the sequence $l_{1,n}, l_{2,n}, \ldots, l_{n,n}$ is log concave which means that

$$l_{k-1,n} l_{k+1,n} \le l_{n,k}^2$$

for all k. We also conjecture that if $i_{n,k}$ is the number of involutions in \mathfrak{S}_n with longest increasing subsequence length k then $i_{1,n}, i_{2,n}, \ldots, i_{n,n}$ is log concave. We show that these two conjectures are strongly related. We also present evidence to support the truth of both. Our main tool is the Robinson-Schensted correspondence. Many other associated conjectures will be discussed.

3.13 Consequences of the no-coincidence assumption in comparative gene order

David Sankoff (University of Ottawa, CA)

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The number of genes in plant and animal genomes tends to exceed 25,000, so that the coincidental gene orders must be very rare unless the genomes have inherited common orders. We discuss two consequences of this. One is the number of chromosomes inferred in an ancestral genome construction, especially in the context of ancient whole genome duplication, where inferring an incorrect number of chromosomes may require unlikely coincidences, The other is the inference of the locus of genome rearrangement on a phylogenetic tree. In this case only certain branches may be inferred to contain a breakpoint, otherwise coincidental changes must have happened. Both of these principles are key to recent reconstructions of ancestral gene orders.

3.14 An Update on Gene Family-free Genome Comparison

Jens Stoye (Universität Bielefeld, DE)

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 Joint work of Daniel Doerr, Louis Antonio Kowada, Jens Stoye, Simone Dantas
 Main reference L. A. B. Kowada, D. Doerr, S. Dantas, J. Stoye, "New Genome Similarity Measures based on Conserved Gene Adjacencies", in Proc. of the 20th Annual Conf. on Research in Computational Molecular Biology (RECOMB'16), LNCS, Vol. 9649, pp. 204–224, Springer, 2016; pre-print available from author's webpage.
 URL http://dx.doi.org/10.1007/978-3-319-31957-5_15
 URL http://www.techfak.uni-bielefeld.de/~stoye/mypublications.html#KOW-DOE-DAN-STO-2016

Many methods in computational comparative genomics require gene family assignments as a prerequisite. While the biological concept of gene families is well established, their computational prediction remains unreliable. In this talk I will present recent results in a new line of research, in which family assignments are not presumed. We study several family-free approaches in detecting conserved structures, genome rearrangements and in reconstructing ancestral gene orders. This leads to a number of interesting combinatorial optimization problems, some of which are easily polynomial-time solvable, while others turn out to be surprisingly hard.

3.15 Positional Constraints for Rearrangements through Noncrossing Colored Partitions and Cycle Packings

Krister Swenson (University of Montpellier 2, FR)

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 Joint work of Krister Swenson, Mathieu Blanchette, Pijus Simonaitis
 Main reference
 K. M. Swenson, M. Blanchette, "Models and algorithms for genome rearrangement with positional constraints", in Proc. of the 15th Int'l Workshop Algorithms in Bioinformatics (WABI'15), LNCS, Vol. 9289, pp. 243–256, Springer, 2015.

 URL http://dx.doi.org/10.1007/978-3-662-48221-6_18

The number of moves is often the sole criterion used to measure the quality of a rearrangement scenario. A current challenge is to incorporate biological information into the gene-order evolutionary model in a manner that is computationally tractable. We present a model amenable towards positional constraints (as seen with chromatin conformation capture data), while elucidating connections between genome rearrangements and noncrossing colored partitions and cycle packings.

3.16 Breaking bad

Eric Tannier (University Claude Bernard – Lyon, FR)

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The permutation as a model for gene order is flawed. It ignores the diversity of susceptibility to breakage across genomic regions, which is necessary even under a uniform random breakage model. I will propose a model of evolution of gene order by inversions where breakage probabilities vary across intergne regions and over time. It contains as a particular

case the uniform breakage model on the nucleotidic sequence, where breakage probabilities are proportional to intergene region lengths. This is very different from the frequently used pseudo-uniform model where all intergene regions have the same probability to break. Estimations of rearrangement distances based on the pseudo-uniform model completely fail on simulations with the truly uniform model. I will propose new combinatorial and statistical problems with this model.

3.17 The substitution decomposition of RNA secondary structures

Vincent Vatter (University of Florida – Gainesville, US)

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 Joint work of Vincent Vatter and Aziza Jefferson

 Main reference A. Jefferson, "The substitution decomposition of matchings and RNA secondary structures", Doctoral dissertation, University of Florida, 2015.
 URL http://gradworks.umi.com/37/29/3729175.html

The substitution decomposition has proved to be a powerful tool for analyzing classes of permutations and of graphs (where it is known as the modular decomposition). I will discuss applications of the substitution decomposition to RNA secondary structures, which can be modeled by matchings.

3.18 On sequence segmentation problems

Tomáš Vinař (Comenius University in Bratislava, SK)

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 Joint work of Martina Višňovská, Tomáš Vinař, Broňa Brejová

 Main reference M. Višňovská, T. Vinař, and B. Brejová, "DNA Sequence Segmentation Based on Local Similarity",
 in Information Technologies – Applications and Theory (ITAT), CEUR Workshop Proceedings,
 Vol. 1003, pp. 36–43, 2013.

 URL http://ceur-ws.org/Vol-1003/

Most rearrangement models work with short segments (called markers, genes, atoms, etc.) that are considered atomic, i.e. they are long enough so that they are identifiable in a genomic sequence and at the same time they are not broken by rearrangement operations. It turns out that precomputing such segments is a difficult and interesting problem, and it is a major obstacle in applying algorithms for rearrangement analyses to real data. In some cases, the problem is in fact equivalent to reconstructing evolutionary history in a given model. In the talk I would discuss several approaches to solving this problem and also include some notes on an approach to analysis of segmental duplications that we have previously introduced.



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