Counting Complexity and Phase Transitions (Spring 2016)

Final Program Report

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Overview

Alan Turing founded the discipline of computability theory. For historical as well as technical reasons the theory is formulated mainly in terms of decision problems. This tradition has been retained for complexity theory, where the most classical complexity classes such as P and NP were defined in terms of decision problems. However for important classes of computations, such as computing probabilities and counting discrete structures, and evaluating a host of well-studied quantities from statistical physics, a more direct perspective is to study computations that produce a numerical quantity, such as those that can be expressed a sum-of-product computation.

These are counting problems in a general sense. The focus of this Simons Institute program was the study of such counting problems, as well as related questions involving the random sampling of combinatorial objects and their typical structure. This included generalizations to weighted counterparts, such as estimating partition functions and sampling from Gibbs distributions. These have been active research topics in Theoretical Computer Science, Statistics and Statistical Physics for some time, but recent years have seen many exciting developments. However, many important problems remain open. The major goal of the program was to coordinate activities between researchers working on these problems, in all areas of exact and approximate counting, and in their applications. While this was the overarching objective of the program, the program activities could generally be grouped into several overlapping sub-topics. A (non-exhaustive) list of these sub-topics follows.

Spin systems and Statistical Physics

A considerable amount of program time was devoted to studying applications to Statistical Physics, as well as applying new ideas that were first suggested as heuristics in physics and attempting to make them mathematically rigorous in the process. Sometimes non-rigorous approaches can suggest interesting phenomena that bring new perspectives to bear on old problems. Of particular interest were problems of mixing in time and space, approximating partition functions, random sampling from Gibbs measures, phase transitions (including those found in random constraint satisfaction problems), and their relationship to computational complexity. The program continued remarkable progress in this area over the past decade.

Markov chain methods

Markov chain Monte Carlo (MCMC) methods have historically provided the most successful approach to approximate counting and estimation of partition functions,

although much recent work has adopted an alternative approach based on spatial mixing. There is no reason to believe that either of these two approaches is uniformly better than the other, and indeed there may even be hope of uniting them. The important applications of the MCMC method, in Statistics and elsewhere, also provided a powerful stimulus to this line of research. The principal interest was in estimation of mixing times for Markov chains of interest, and techniques for performing estimations from them. This line of work also includes sampling algorithms that are closely related to approximate counting.

Homomorphisms and CSPs

There has been spectacular progress in recent years in establishing the computational complexity of the general task of counting the number of solutions to Constraint Satisfaction Problems (CSPs). The leading figures in these developments were all long-term participants in the program. In the exact counting case, this work has resulted in very general dichotomy theorems, which completely classify broad classes of problems into those that are tractable and those that are intractable. For approximate counting, such dichotomy theorems appear unlikely, but substantial progress on classification has been made. Significant new results in both exact and approximate counting were obtained during the program. A further interest was in the study of random CSPs and thresholds for existence of solutions. Impressive progress has been made recently in this area, and was continued during the program.

Holant problems

The study of the holant, and holographic algorithms for computing it, was initiated by Valiant. It is a far-reaching generalization of graph matchings, and can also be viewed as an edge-based variant of the (vertex-based) CSP. The gadgets used are matchgates and their variants, and these have proved useful both algorithmically and in proofs of hardness. While establishing a complete classification for the complexity of computing the general holant appears more difficult than for counting CSPs, significant results have been obtained in restricted cases. Most results have been obtained for the Boolean case with symmetric signatures, but attention is now being directed towards higher domain problems and asymmetric signatures. Notable progress in these areas was made during the program.

Review of Program Activities

By any reasonable measure, the program was a resounding success. This is reflected not only in the significant list of publications it has already produced in high-impact conferences and journals, such as the *IEEE Symposium on Foundations of Computer Science (FOCS)*, the ACM Symposium on the Theory of Computing (STOC), the ACM-SIAM Symposium on Discrete Algorithms (SODA), the International Colloquium on Automata, Languages and Programming (ICALP), the Journal of the ACM and *SIAM Journal on Computing*, but also in establishing a more collaborative research agenda that spans the whole of the counting program, and in fostering long term research connections among the program participants.

The program started with a Boot Camp, as is the usual practice for Simons Institute programs, the purpose of which was to bring various participants of different backgrounds together and to present an overview of the scope and thrust of the program. Judging by the feedback from the participants, this was quite a success. Of particular note was the uniformly high standard of the presentations by the speakers, who obviously took a good deal of effort in their preparations. The Boot Camp was designed to involve many of the younger long-term participants, and they communicated their enthusiasm as well as their knowledge. This Boot Camp set the tone for the rest of the program in a most collaborative spirit.

The semester-long program also hosted three workshops: "Approximate Counting, Markov Chains and Phase Transitions", Feb. 22 – Feb. 26, 2016; "The Classification Program of Counting Complexity", Mar. 28 – Apr. 1, 2016; and "Random Instances and Phase Transitions", May 2 – May 6, 2016. These workshops were well attended, not only by long-term program participants, but also by invited speakers and others from outside the program who self-registered. The commonality with the parallel program on "Algorithmic Challenges in Genomics" was also reflected in the attendance at workshops and seminars, though research interaction with that program took place mostly on an individual basis. The program also organized a reunion workshop at the one-year anniversary, in May 2017, to report on the progress made and to reflect on the challenges ahead. From the talks and discussions at the reunion workshop it was clear that a great deal of progress was either made directly during, or initiated at the Simons Institute by people who were brought together by the program.

The program had one weekly seminar, on Friday afternoons, organized by Andreas Galanis and Heng Guo. This had a steady stream of interesting talks, which were always well attended. In addition, three informal working groups were established within the program. The working group on phase transitions in random instances was organised by Lenka Zdeborova; a group on proving stronger results in counting complexity under stronger complexity assumptions (mainly the Exponential Time Hypotheses) was organized by Radu Curticapean and Holger Dell; and a group on relationships between counting and quantum computing was organized by John Lapinskas and Steve Homer. These groups were lively and well attended, and continued meeting throughout the program.

There were two Open Lectures, directed at the larger UC Berkeley campus community. The first lecture (by Alan Frieze of Carnegie-Mellon University) gave an overview of phase transitions in random structures, which was an important theme of the program. The second (by Leslie Valiant of Harvard University) covered holographic algorithms and holographic reductions for proving complexity results. Again, this reflected an important theme of the program. Both attracted sizable audiences, and appeared to be well received.

There was also an active social program, organized by the staff of the Institute and longterm participants Holger Dell and John Lapinskas. This involved, inter alia, afternoon teas, receptions at the Institute, group walks, outings to concerts and films, and a weekly board games evening. This helped to give an air of collegiality to the program, particularly amongst the younger participants.

Research interactions were mostly conducted at an informal level in the many collaboration spaces at the Institute, in addition to the formal seminars and workshops described earlier. Judging from the excellent research results obtained by the program participants, as documented in numerous journal and conference publications as well as in the individual research reports submitted by participants at the time of the reunion workshop, it is clear that these informal interactions were extremely productive, and resulted in some of the most striking advances of the program.

Research Outcomes

The program made significant progress in all areas of its proposed research activity. We now briefly describe several major results that were achieved by program participants. A common theme was that these advances were made possible by bringing the participants together for an extended period at the Institute. This is by no means an exhaustive list of achievements, but is intended to give some examples and highlights. Several of these papers have been accepted for presentation at flagship conferences such as the IEEE FOCS and ACM STOC.

There was great interest in developing rigorous versions of the one-step replica • symmetry breaking and belief propagation methods from Statistical Physics for random combinatorial problems. Recent work has made substantial progress in understanding the phase transitions in random constraint satisfaction problems. In particular, for several of these models, the exact satisfiability threshold has been rigorously determined, confirming predictions of statistical physics. A particular breakthrough in this area coming out of the program was paper [116] (presented at FOCS 2016) by Allan Sly, Nike Sun and Yaming Zhang on the number of solutions for random regular NAE-SAT. In this work the authors gave a complete solution throughout the condensation phase where earlier methods had failed. A substantial portion of the work was carried out during the program and benefited from insights from the statistical physicists who were also present as long-term visitors. The authors consider random regular k-NAE-SAT: knowing the satisfiability threshold, it is natural to study, in the satisfiable regime, the number of solutions of a typical instance. They prove that these solutions have a welldefined free energy (limiting exponential growth rate), with an explicit value matching the one-step replica symmetry breaking prediction from physics. The

proof develops new techniques for analyzing a certain "survey propagation model" associated to this problem. It is believed that these methods may be applicable to a wide class of related problems.

- In a similar vein, as reported at the reunion workshop, a chain of collaborative research resulted in a proof of a conjectured formula for the mutual information in statistical inference problems induced by random graphs (paper [51], which appeared recently in STOC 2017) by Amin Coja-Oghlan, Florent Krzakala, Will Perkins and Lenka Zdeborova. Early in the program, Zdeborova and Krzakala felt that the Guerra interpolation method can lead to a rigorous derivation of the replica results (that they had developed previously) for a class of Bayes-optimal inference problems. Then they talked to Jiaming Xu, another program participant whom they met at the Institute, and through discussions they realized that a proof for one side of the bound can indeed be obtained. This resulted in the joint paper [100]. Then as a follow up they realized, with Nicolas Macris who was visiting for the third workshop of the program, that they could also work out the converse bounds, resulting in paper [7]. Finally, Zdeborova and Krzakala also met Perkins during his visit to the Institute and realized that their results in [100] and [7] on dense systems could can be extended to sparse systems, which finally led to paper [51]. This paper is also concerned with the cavity method, and the quest to make various predictions of it rigorous. The result established in the paper implies a well-known conjecture by Decelle et al., and allows a precise pinpointing of the condensation phase transition in random constraint satisfaction problems such as random graph coloring. The proof provides a conceptual underpinning of the replica symmetric variant of the cavity method.
- Jin-Yi Cai and his collaborators produced some comprehensive results in the • classification program of the complexity of exact counting. With Zhiguo Fu, he showed that holographic algorithms with matchgates are universal for planar #CSP over the Boolean domain. This work was presented in the 2017 STOC [41], and the full paper runs to about 100 pages. They proved the following sweeping classification theorem that classifies all counting constraint satisfaction problems (#CSPs) over Boolean variables into exactly three categories: (1) Polynomial-time tractable; (2) #P-hard for general instances, but solvable in polynomial-time over planar graphs; and (3) #P-hard over planar graphs. The classification applies to all sets of local, not necessarily symmetric, constraint functions on Boolean variables that take complex values. It is shown that Valiant's holographic algorithm with matchgates is a universal strategy for all problems in category (2). This completely resolves the question, in the #CSP framework over the Boolean domain, about the power of Valiant's holographic algorithms. The remaining challenge is for the holant problem, where known classification theorems only apply to symmetric constraint functions. As a first step in achieving a holant dichotomy, Cai in collaboration with Zhiguo Fu and Mingji Xia gave a

complexity classification for the six-vertex model, which is of independent interest in the physics community and has been well studied for many decades. As reported in the reunion workshop, they have extended the classification to the planar case of the six-vertex model, as well as to the eight-vertex model. These are base cases in a potential inductive proof for a general holant dichotomy. Also in preparation for the classification of holant problems, Cai, Pinyan Lu and Mingji Xia achieved a complexity dichotomy for holant^c over the Boolean domain, that had eluded them for at least five years. The breakthrough was the discovery of a new class of tractable holant^c problems, specified by local affine functions. These are reported in papers [40,42,43,45]. Also, a book by Cai and Xi Chen, "Complexity Dichotomies for Counting Problems" was finally finished during the Simons Institute program, and will be published by Cambridge University Presss in September 2017.

Alexander Barvinok pioneered a new approach to deriving deterministic algorithms for approximating partition function polynomials via Taylor series expansions. This approach is discussed in detail in his recent book [9], which was completed during his stay at the program. Indeed, Barvinok reports on extensive discussions with Guus Regts at one of the workshops that were very helpful to him in completing his book. Soon after the semester ended, Patel and Regts made substantial progress in transforming quasi-polynomial interpolation algorithms based on Barvinok's approach into genuinely polynomial ones on bounded degree graphs, and then Peters and Regts proved Sokal's conjecture on the roots of the independence polynomial of a graph. For Barvinok, this last result was a vindication of the interpolation approach, as it allows the method to match Weitz's complexity bound for the approximation of the independence polynomial. The original method gives only pseudo-polynomial time algorithms, but further developments by Patel and Regts, and by Liu, Sinclair and Srivastava [104] (all participants in the program) have refined this to give polynomial time algorithms in certain important cases, including the ferromagnetic Ising model. In particular, the work of Liu, Sinclair and Srivastava [104] gives the first deterministic approximation algorithm (FPTAS) for the ferromagnetic Ising partition function for bounded degree graphs that works throughout the range of parameter values except at zero field. Previous algorithms have either been randomized (MCMC), or have worked only in the uniqueness regime. Their approach combines the work of Barvinok and Patel and Regts metioned above, together with the classical Lee-Yang theorem, which localizes the zeros of the Ising model partition function. They extend their results to hypergraphs, proving along the way an extension of the Lee-Yang theorem to hypergraphs, and to general ferromagnetic two-spin systems.

- Solving CNF formulas (Boolean formulas in Conjunctive Normal Form) is one of ٠ the central problems in computer science, and the Simons program led to new progress on the computational complexity transition in counting/sampling solutions to a CNF formula. Suppose each clause in the formula has k literals, and each variable appears in at most d clauses. The classical Lovasz Local Lemma, and its later algorithmic version due to Moser and Tardos, have established an easy-to-hard transition at around $d = 2^k$ for deciding/searching for a solution. However, the previously best known algorithm for counting/sampling has only a linear dependency between k and d, and hardness results were known around d = $2^{k/2}$. During the program, Hermon, Sly and Zhang [93] (all long-term participants of the program) found a new argument to analyze the mixing time of Glauber dynamics in monotone formulas, establishing a rapid mixing bound on $d \le c 2^{k/2}$ which is tight up to constants. Independently, Guo, Jerrum and Liu (also longterm program participants: Guo was a Research Fellow and Liu a graduate student) found a new sampling algorithm called "partial rejection sampling", which can be applied to any constraint sampling problem, and whose running time is stochastically dominated by that of rejection sampling. Their paper [84], presented at STOC 2017, proposed a new algorithmic framework that connects the algorithmic Lovasz Local Lemma and uniform sampling. Applied to CNF formulas, this new algorithm is efficient under an almost tight dependency between d and k, though under some additional min-intersection conditions. (Interestingly, yet another concurrent and independent contribution was made by Moitra, outside the program, who gave an algorithm that works with a (not tight) exponential dependency between d and k, with no additional conditions.) Although the sharp transition threshold for sampling CNF solutions remains elusive, these exciting new developments have greatly enhanced our understanding and provided new tools to attack this important problem.
- Research Fellow Radu Curticapean produced an impressive stream of work on • counting graph matchings. This produced papers on matchings with k unmatched vertices in planar graphs [58], on a new "parity separation" method for weighted matchings [59], on counting edge-injective homomorphisms and k-matchings in restricted graph classes (with Holger Dell and Marc Roth) [62], and on tight conditional lower bounds for counting perfect matchings on graphs of bounded treewidth, cliquewidth and genus (with Dániel Marx) [63]. In a breakthrough in late 2016, in joint work with Research Fellow Holger Dell and Dániel Marx, they managed to unify several disparate branches of parameterized counting complexity by introducing so-called "graph motif parameters": these are graph parameters that count small structures in graphs. Formally, fix a graph H and let #Ind(H->*) denote the function that maps input graphs to the number of induced H-copies appearing in them. A graph motif parameter is any function that can be written as a finite linear combination of such basis functions, involving a finite set of graphs H. This encompasses essentially all problems that ask to count some

kind of small pattern in graphs, including those that were defined previously in [62]. They developed new algorithms for computing graph motif parameters on input graphs (in many cases these are now the fastest algorithms known, e.g., for counting k-matchings or k-paths). They also gave a full dichotomy for the complexity of evaluating graph motif parameters: if one fixes a recursively enumerable class of graph motif parameters, evaluating some f from this class is either FPT in the description length of f, or #W[1]-hard. The resulting paper [61] appeared at STOC 2017.

- Work on applying the correlation decay methods from Statistical Physics to problems of approximate counting was done by Ivona Bezáková, Andreas Galanis, Leslie Goldberg, Heng Guo, and Daniel Štefankovič, who showed that these methods can be applicable even when strong spatial mixing fails [16].
- Other notable work on Markov chain Monte Carlo was done by Antonio Blanca and Alistair Sinclair [19,20], and by Heng Guo and Mark Jerrum [83] on the random-cluster model; by Nayantara Bhatnagar and Dana Randall on simulated tempering and swapping in mean-field models [18]; and by Colin Cooper, Martin Dyer, Catherine Greenhill and Andrew Handley on the flip Markov chain for connected regular graphs [54]. This last paper introduces a two-stage canonical path method for Markov chain analysis, which appears superior to the classical Diaconis and Saloff-Coste comparison method whenever that is applicable.
- Charilaos Efthymiou, Tom Hayes, Daniel Štefankovič, Eric Vigoda and Yitong Yin produced some very interesting work on the convergence of MCMC and loopy belief propagation in the tree uniqueness region for the hard-core model. This work, which appeared in the 2016 FOCS conference [69], seeks to combine the belief propagation and MCMC methods to achieve the best of both worlds. This may well provide an important direction for future research.
- Andreas Galanis, Leslie Goldberg and Mark Jerrum proved a trichotomy theorem for the complexity of approximately counting graph homomorphisms [79].

Concluding Remarks

Overall, the program on "Counting Complexity and Phase Transitions" was a great success. It covered a variety of topics, building on the core topic areas in the proposal as well as some newer developments, such as the structure of random CSPs and the algorithmic Lovasz Local Lemma. It fostered a great collaborative research environment. Substantive collaborations from people across subareas in the field resulted in a number of notable successes as outlined above. As evidenced by publications that have already appeared within one year of the program, as well as others in the pipeline, many of which

were presented during the reunion workshop, new collaborations have been fruitfully established. Many of these research collaborations are direct results of the program, without which they are unlikely to have happened. As the main organizers, we feel that the accomplishments of the program have made our experience organizing it a fond memory and a worthwhile service to the community. And of course, the leadership and the staff members at the Simons Institute made it all possible; we extend our thanks to them.

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