Computational Complexity and Partition Functions

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— Abstract -

This paper is an extended abstract of my STACS 2019 talk "Computational Complexity and Partition Functions".

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1 Extended Abstract and Annotated Bibliography

A partition function is a polynomial which summarises properties of physical systems such as spin models (for example – the Ising model, the Potts model, the hard core model, or the monomer-dimer model). The talk does not assume knowledge of these models. The goal in the research area is to develop good approximation algorithms for partition functions, and to understand, in terms of the parameters of the models, when the partition functions can be (approximately) evaluated. Typically, a partition function is represented implicitly by a (small) graph, but it has exponentially many terms, so evaluation is non-trivial.

This talk is a survey, designed to introduce results, methods, and open problems in the area. An emerging trend is that, in order to really understand partition functions, it is useful to work over complex numbers, rather than just over the reals. This written extended abstract does not discuss methods – it is meant to serve more as an annotated bibliography – helping somebody who attended the talk to find the relevant papers.

The talk will start by introducing the independence polynomial of a graph, which is the partition function of the hard core model. This is a model of a gas whose particles occupy the vertices of a graph. Particles have non-negligible size (so cannot be adjacent). The model has a parameter λ . The partition function is given by $Z_G(\lambda) = \sum_{I \in \mathcal{I}_G} \lambda^{|I|}$, where \mathcal{I}_G is the set of independent sets of a graph G and |I| is the number of vertices in the independent set I. We will consider the problem of approximating $Z_G(\lambda)$, given a graph G with maximum degree at most Δ .

When λ is a real number, much is known. In particular, the complexity of approximating $Z_G(\lambda)$ is completely captured by two real-valued thresholds λ^* and λ_c which depend on Δ and satisfy $0 < \lambda^* < \lambda_c$. In the positive direction, $Z_G(\lambda)$ is efficiently approximable if λ is in the interval $(-\lambda^*, \lambda_c)$ [8, 11, 15, 16].

Outside of the interval $[-\lambda^*, \lambda_c]$, subject to suitable complexity-theoretic assumptions, no efficient approximation algorithm exists [7, 14]. The talk will discuss the relevance of

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the thresholds $-\lambda^*$ and λ_c . In fact, these are the two real points on the boundary of a cardiod-shaped region in the complex plane [12] which is the region in which the "occupation ratio" at the root of a Δ -regular tree converges, as the height of the tree grows. (This means that, for parameters λ inside this region, when we consider the model on a Δ -regular tree, the contribution to the partition function from independent sets in which the root is occupied converges to some fixed fraction of the value of the total partition function.) Peters and Regts naturally asked whether this cardiod coincides with the region where efficient approximation is possible. It is now known [5] that efficient approximation is impossible outside of the cardiod (subject to complexity-theoretic assumptions). Inside the cardiod, there are many regions where we do have efficient approximation algorithms [4, 8, 11, 12] but the full picture is not fully resolved, so there are plenty of open questions.

Another interesting partition function is the matching polynomial of a graph, which is the partition function of the monomer dimer model. A "monomer" is an unmatched vertex in a matching, and a "dimer" is a pair of matched vertices. The model has a parameter γ and the partition function is given by $Z_G(\gamma) = \sum_{M \in \mathcal{M}_G} \gamma^{|M|}$, where \mathcal{M}_G is the set of matchings of a graph G and |M| is the number of edges in a matching M. When γ is a positive real, there is an efficient randomised approximation algorithm based on Monte Carlo simulation [10]. The applicability of *deterministic* approximation is fully resolved for bounded-degree graphs. It turns out that this is possible for any γ except (subject to complexity assumptions) when γ is a real number less than $-1/(4(\Delta-1))$ [3, 6, 11]. The reason that approximation is impossible for these values of γ (and possible elsewhere) is to do with the fact that this is where the zeroes of the polynomial are located [9]. In general, the method of Barvinok [1, 2] leads to efficient approximation algorithms in complex domains where there are no roots, but in turn, the existence of roots sometimes leads to provable intractability. The approximability question has also been investigated when the bounded-degree requirement is relaxed to a notion of average degree, namely the connective constant. For graphs with bounded connective constant, it turns out that efficient approximation is possible everywhere except when γ is a negative real. Moreover, there is a set of values which is dense on the negative real axis where efficient approximation is impossible (subject to complexity assumptions) [6, 13].

There are many interesting partition functions, such as the partition functions of the Ising model and the Potts model, that will not be discussed in the talk. The chosen examples are designed to give a taste of results, methods and open problems in this research area.

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