ARC Proposal: Phase Transitions in the Complexity of Counting

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Motivation

The problem of estimating the partition function for the hard-core lattice gas model on finite graphs has a striking phase transition in its computational complexity that has a remarkable connection to phase transitions in the model on infinite trees. For a graph G = (V, E) and activity $\lambda > 0$, the hard-core model is defined on the set $\mathcal{I}(G)$ of independent sets of G where a set $I \in \mathcal{I}(G)$ has weight $w(I) := \lambda^{|I|}$. The so-called partition function for the model is defined as:

$$Z_G(\lambda) := \sum_{I \in \mathcal{I}(G)} w(I) = \sum_{I \in \mathcal{I}(G)} \lambda^{|I|}.$$

Finally, the Gibbs distribution μ is over the set $\mathcal{I}(G)$ where $\mu(I) = w(I)/Z_G(\lambda)$. Sampling from the Gibbs distribution is necessary for running simulations, and estimating the partition function is necessary for estimating certain thermodynamic properties of the system.

The notion of the partition function gives rise to the counting problem of computing the value $Z_G(\lambda)$. Since it is NP-hard to exactly compute the partition function [11], even for graphs with maximum degree equal to 3 [4], the computational complexity of approximating the partition function has received extensive attention. Note, an efficient algorithm for approximating the partition function yields an efficient scheme for (approximately) sampling from the Gibbs distribution [6].

In this direction of approximating the partition function, it was not until recently that an important computational transition was established. Namely, Weitz [12] gave an FPAS (fully polynomial-time approximation scheme) for the partition function of graphs with maximum degree Δ when Δ is constant and $\lambda < \lambda_c(\Delta) := (\Delta - 1)^{\Delta - 1}/(\Delta - 2)^{\Delta}$. On the other hand, Sly [10] proved that, unless NP = RP, for every $\Delta \geq 3$, there exists an $\varepsilon(\Delta) > 0$ such that for graphs with maximum degree Δ there does not exist an FPRAS (fully-polynomial time randomized approximation scheme) for the partition function at activity λ with $\lambda_c(\Delta) < \lambda < \lambda_c(\Delta) + \varepsilon(\Delta)$. In a recent joint work [1], we extended Sly's inapproximability result for all values of λ with $\lambda > \lambda_c(\Delta)$ except for the cases $\Delta = 4, 5$.

This computational transition is even more interesting in light of the fact that it coincides with the phase transition on the infinite Δ -regular tree \mathbb{T}_{Δ} . Formally, the activity $\lambda_c(\Delta)$ is also the critical activity for the uniqueness/non-uniqueness of infinite-volume Gibbs measures on \mathbb{T}_{Δ} [7]. Roughly speaking, the phase transition on \mathbb{T}_{Δ} captures whether root to leaves correlations persist or decay exponentially as the depth of the tree goes to infinity. In summary, the results of [10], [12] (and [1]) establish a computational phase transition for general graphs that coincides exactly with the statistical physics phase transition on trees.

The question which arises is whether there are other models which exhibit a similar correspondence between computational hardness and phase transitions. In this vein, the Ising model is a particularly interesting model to study since it is the classical model in statistical physics, and the above results for the hard-core model suggest that a similar phenomenon might hold for the Ising model.

Approximating the Partition Function in the Ising model

The Ising model is used to study the magnetization of a solid. For a graph G = (V, E), a configuration is defined as an assignment $\sigma : V \to \{-1, +1\}$. For a given configuration $\sigma \in \{-1, +1\}^V$, denote by $m(\sigma)$ the number of edges whose both endpoints are assigned the same value. For simplicity here, we define the model for the case of no external field, which is arguably the more interesting setting.

The Ising model on G with (inverse) temperature β is defined on the set of all configurations $\{-1,+1\}^V$, where a configuration $\sigma \in \{-1,+1\}^V$ has weight $w(\sigma) = \exp(\beta m(\sigma))$. The partition function for the model is then defined as $Z_G(\beta) := \sum_{\sigma \in \{-1,+1\}^V} w(\sigma) = \sum_{\sigma \in \{-1,+1\}^V} \exp(\beta m(\sigma))$. The Gibbs distribution μ is over the set $\{-1,+1\}^V$ where $\mu(\sigma) = w(\sigma)/Z_G(\beta)$.

The Ising model exhibits a qualitative difference with respect to the value of β . Namely, if $\beta > 0$ the model is called *ferromagnetic* since assignments with the same values at the endpoints of an edge are favored, whereas if $\beta < 0$ the model is called *anti-ferromagnetic* since assignments with different values at the endpoints of an edge are weighted higher.

We are interested in the computational complexity of approximating the partition function of the Ising model. Jerrum and Sinclair [5] have designed an FPRAS for the ferromagnetic Ising model on graphs of arbitrary degree. Hence, our focus is on the anti-ferromagnetic Ising model. Our goal in this project is to prove the following conjecture that we make:

Conjecture 1. For the anti-ferromagnetic Ising model, let $\beta_c(\Delta) := \ln\left(\frac{\Delta-2}{\Delta}\right)$ denote the critical temperature for the phase transition of uniqueness/non-uniqueness on the infinite tree \mathbb{T}_{Δ} . For all graphs G of maximum degree Δ , for all $0 > \beta > \beta_c(\Delta)$, when Δ is constant, there is an FPAS for approximating the partition function. For all $\Delta \geq 3$, for all $\beta < \beta_c(\Delta)$, unless NP = RP, there does not exist an FPRAS for approximating the partition function.

We briefly describe results in literature which are linked to Conjecture 1. First, the uniqueness regime of Gibbs measures for the Ising anti-ferromagnetic model on the infinite Δ -ary tree is well-known [2]. Second, the work of Sinclair *et al.* [9]), building upon Weitz [12], yields an FPAS for the anti-ferromagnetic Ising model in the uniqueness regime of the infinite Δ -ary tree, when Δ is constant, thus establishing the approximability side of the conjecture.

For the inapproximability side of the conjecture, there are results known (e.g., [3]), but they are far from matching the critical point $\beta_c(\Delta)$. To obtain tight results, we will look to the approach of Sly [10] for the hard-core model. In this regard, our recent work [1] which improves Sly's results gives us confidence that we can address this problem.

In [1] the main result is an improvement in the result of [8]. In [8], they prove that for the hard-core model, for the same range of λ as in Sly's inapproximability result, the Glauber dynamics (which is a simple single-site Markov chain for sampling from the Gibbs distribution) is torpidly mixing (i.e., it takes exponentially long in |V| to converge to its stationary distribution) on random regular graphs with high probability. This torpid mixing result is a main component in Sly's proof. The proof of this torpid mixing result involves a technically complicated second moment argument. In [1] we improve this second moment argument to obtain our improved result. Our first goal in this project will be to establish an analogous torpid mixing result for the anti-ferromagnetic Ising model on random regular graphs. We will then aim to use that torpid mixing result to obtain the inapproximability result conjectured above for all $\beta < \beta_c(\Delta)$. Finally, if we can establish Conjecture 1, we will explore the phenomenon for more generalized versions of the Ising model (such as those considered in [3] and [9]), to get a more clear picture for what models there is a computational phase transition as for the hard-core model, and for what models there is an efficient algorithm for estimating the partition function for all temperatures as for the ferromagnetic Ising model [5].

References

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