Subgraphs-world Process in the Ising Model

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Abstract

The physics of phase transitions can be modeled by an arrangement of sites in a d-dimensional lattice known as the Ising model, in which each site is assigned either a positive or negative spin. In this paper, we will first provide an introduction to the Ising model. We will define the partition function of an Ising system, and present the problem of its computation.

In 1993, Jerrum and Sinclair developed a revolutionary new approximation algorithm for the partition function of an arbitrary ferromagnetic Ising system. The key innovation Jerrum and Sinclair presented is a new Markov chain known as the Subgraphs-world model from which we can sample random states of the Ising system. The Subgraphs-world chain proves to be rapidly mixing, which allows us to efficiently approximate the partition function through sampling. We will introduce the chain, and show that it is rapidly mixing.

1 Introduction

The Ising model consists of a collection of sites $[n] = \{0, 1, \ldots, n-1\}$. Each pair of sites i, j has an associated interaction energy V_{ij}. We call the set of pairs with nonzero interaction energies E, and this set forms a regular lattice graph $([n], E)$. We define a configuration to be an assignment of positive ($\sigma_i = +1$) and negative ($\sigma_i =$ -1) spins to each site $i \in [n]$. A given configuration has energy given by the Hamiltonian

$$H(\sigma) = -\sum_{\{i,j\}\in E} V_{ij}\sigma_i\sigma_j - B\sum_{k\in[n]} \sigma_k,$$

where B is a number that reflects the size of the external field.

A special case of the Ising model occurs when all interaction energies are nonnegative. The system then models the behavior of a ferromagnet, further detailed in Cipra's paper [1].

In a more general system, our chief goal in working with the Ising model is to compute the partition function, given by

$$Z = Z(V_{ij}, B, \beta) = \sum_{\sigma} \exp\left(-\beta H(\sigma)\right),$$

where β is related to temperature and the sum runs over all possible configurations σ. Knowledge of Z allows us to compute most of the relevant physical properties of the system. Most importantly, the probability that the system in equilibrium is found in configuration σ is given by $\exp\left(-\beta H(\sigma)\right)$. Other quantities such as the mean energy and the mean magnetic moment correspond to certain logarithmic derivatives of Z. Additionally, phase transitions in the system generally correspond to singularities in these derivatives.

2 Markov Chains and the Ising Model

The logic behind using Markov chains in computing the partition function is that in order to compute weighted combinatorial sums, it often suffices to be able to sample configurations at random with probabilities proportional to their weights. In the case of the Ising model, we sample over all configurations σ with weights $\exp\left(-\beta H(\sigma)\right)$. The goal is to set up an ergodic Markov chain with configurations as its states and with transitions that correspond to small local perturbations in the system. If we can then design the chain so that its equilibrium distribution is the appropriate weighted distribution over all configurations, then we can perform a random sampling by running the chain for a certain number of steps and taking whatever state it ends up in. The catch, however, is that unless the chain used is rapidly mixing, this procedure might be highly inefficient. The first attempts made by physicists to apply this procedure utilized Markov chains on the Ising spin configurations σ. Unfortunately, no such chains were found to be rapidly mixing for all possible parameter values.

3 Subgraphs-world Process

Along come Jerrum and Sinclair, whose Markov chain makes use of an entirely new domain where the configurations are spanning subgraphs of the interaction graph $([n], E)$. We determine an energy for each subgraph using weights attached to its edges and vertices. Though the physical significance of these subgraph configurations is not clear, the partition function of this

chain is very closely related to that of the chains on spin configurations σ. Most importantly, we are able to define a natural chain on these subgraphs with the desired equilibrium distribution which is rapidly mixing. The Markov chain, $\mathcal{MC}_{Ising}$ of the subgraphs-world process is defined as follows. The state space Ω is the set of all spanning subgraphs $X \subseteq E$. We note that $|\Omega| = 2^m$, where $m = |E|$ is the number of unordered pairs $\{i, j\}$ with nonzero interaction energy.

For X, $X^{'} \in \Omega$ with $X \neq X^{'}$, the transition probability from X to $X^{'}$ is given by

$$p(X, X^{'}) = \begin{cases} 1/2m & \text{if } |X \oplus X^{'}| = 1 \text{ and } w(X^{'}) \geq w(x) \\ w(X^{'})/2mw(X) & \text{if } |X \oplus X^{'}| = 1 \text{ and } w(X^{'}) < w(x) \\ 0 & \text{otherwise,} \end{cases}$$

where $X \oplus X^{'}$ denotes the symmetric difference of X and $X^{'}$. Here, $w(X)$ is the weight assigned to a given configuration $X \subseteq E$.

4 Rapid Mixing

To show that their chain is rapidly mixing, Jerrum and Sinclair make use of two theorems. To understand the first theorem, we need to define a measure known as conductance.

For an ergodic reversible Markov chain, the conductance is defined by

$$\Phi = \min \left\{ \sum_{\substack{X \in S \\ X^{'} \notin S}} q(X, X^{'}) / \sum_{X \in S} \pi(X) \right\}$$

where the minimization is over all subsets S of states with $0 < \sum_{X \in S} \pi(X) \leq 1/2$. Conductance serves to measure the rate at which the Markov chain moves around the state space. Given that the chain starts in some state in some small subset S of the state space, the conductance provides a lower bound on the conditional probability that the stationary process gets out of S in a single step. Thus, we might expect a chain with a large conductance to converge fast.

Theorem 1. Let Φ be the conductance of an ergodic, reversible Markov chain with stationary distribution π and $\min_X p(X, X) \leq 1/2$. Let $p^{(t)}$ denote the distribution of the state at time t given that the initial state is X_0. Then the variation distance $||p^{(t)} - \pi||$ satisfies

$$||p^{(t)} - \pi|| \leq \frac{(1 - \Phi^2)}{\pi(X_0)}.$$

The full proof of Theorem 1 can be read in Jerrum and Sinclair's paper [2], but we will outline some key points here. Jerrum and Sinclair showed that the variation distance at time t is related to the second eigenvalue λ_1 of the Markov chain by the inequality

$$||p^{(t)} - \pi|| \leq \frac{\lambda_1^t}{\pi(X_0)}$$

.

Additionally, Jerrum and Sinclair show that the bound

$$\lambda_1 \leq 1 - \Phi^2$$

holds for chains in which all self-loop probabilities are at least 1/2. Theorem 1 results from these two inequalities. The converse of Theorem 1 states that the conductance of a rapidly mixing Markov chain cannot be too small. In order to ensure a variation distance of at most δ, it is sufficient to run the chain for $\Phi^2(\ln \delta^{-1} + \ln \pi(X_0)^{-1})$ steps. So if the conductance has an inverse polynomial lower bound, then rapid mixing will generally follow. We provide such a bound for the $\mathcal{MC}_{Ising}$ chain with the following theorem.

Theorem 2. The conductance of the Markov chain $\mathcal{MC}_{Ising}$ is bounded below by $\mu^4/4m$.

A full proof of Theorem 2 can be read in Jerrum and Sinclair's paper [2], but we will outline their method here. They develop a general path counting argument, which can then be applied to the $\mathcal{MC}_{Ising}$ chain.

For each pair of states $I, F \in \Omega$, we specify a canonical path from I to F, i.e. from the initial state to the final state. Each step along the canonical path is performed using a valid transition of the Markov chain. We assign a weight to each canonical path, determined by the product of the stationary probabilities at the initial and final states. So the weight of the path from I to F is given by $\pi(I)\pi(F)$, and is independent of the intermediate states along the path. The logic is that if we choose these canonical paths well, we will be able to produce a good bound on conductance. We suppose that we can show that for each transition $T \to T^{'}$, the aggregated weight of all canonical paths of which the transition $T \to T^{'}$ occurs is bounded above by $bq(T, T^{'})$, where $q(X, X^{'}) = \pi(X)p(X, X^{'})$. We will consider any partition of the state space into two sets S and $\bar{S}$ such that $\sum_{X \in S} \pi(X) \leq 1/2$. Thus the total weight of all canonical paths which cross the cut defined by S and $\bar{S}$ is at least

$\sum_{I \in S} \sum_{F \in \bar{S}} \pi(I)\pi(F) = \pi(S)\pi(\bar{S}) \geq \pi(S)/2$. Additionally, when we sum over all transitions $T \to T^{'}$ with $T \in S$ and $T^{'} \in (\bar{S})$, we get that the total weight of all canonical paths which cross the cut is bounded above by $b \sum_{T \in S} \sum_{T^{'} \in (\bar{S})} q(T, T^{'})$. And since S and $(\bar{S})$ represent a general partition of the state space, we may conclude that the Markov chain's conductance is bounded below by $1/2b$. The bulk of the proof involves estimating b, which is then used to obtain a bound on conductance, and hence the rate of convergence of the chain $\mathcal{MC}_{Ising}$.

5 Conclusion

With the innovation of the rapidly mixing Markov chain of the Subgraphs-world model, Jerrum and Sinclair developed the first provably efficient approximation algorithm for the partition function of an arbitrary Ising system. Their algorithm runs in time polynomial in the number of sites n. Jerrum and Sinclair also show in their paper that their algorithm is essentially the best one can hope for [2]. The problem of computing the partition function for the Ising model, when viewed as a combinatorial enumeration problem, turns out to be #P-complete, which is also further detailed on in the Jerrum and Sinclair paper [2].

References

[1] B. Cipra (1987), An introduction to the Ising model, Amer. Math. Monthly, 94, 937-959.

[2] M. Jerrum and A. Sinclair (1993), Polynomial-time approximation algorithms for the Ising model, SIAM Journal on Computing, 22, 1087-1116.