Sampling Spin Configurations of an Ising System

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Abstract. We present the first provably polynomial time sampling scheme for generating spin configurations of any ferromagnetic Ising system, one of the most widely studied models in statistical mechanics. The algorithm is based on the randomized approximation scheme of Jerrum and Sinclair which estimates the partition function of the Ising system using the so-called "high temperature expansion" representation. Their estimation algorithm did not give rise to an Ising sampling algorithm via self-reducibility because ferromagnetism was not preserved by the reductions. Recently Nayak, Schulman and Vazirani gave a quantum algorithm for sampling Ising spin states based on the JS algorithm. We show that by using the JS algorithm and a third equivalent representation of the Ising partition function (the Fortuin-Kasteleyn "random-cluster model"), self-reducibility yields a (classical) polynomial time algorithm for sampling Ising spin configurations.

A *ferromagnetic Ising system* (see [2] for a general introduction) consists of a graph G whose vertices represent particles and whose edges represent interactions between particles. A spin configuration is an assignment of *spins*, either 0 or 1, to each of the particles. Particles which are adjacent prefer to have the same spin. In addition, there may be an external magnetic field which makes each vertex prefer one of the two spins. A standard reduction replaces this field by an extra spin variable, so for convenience we assume without loss of generality that the external field is zero. More precisely, let $J_{x,y}$ be the interaction energy between vertices x and y, where $(x,y) \in E$. In a ferromagnetic Ising system, $J_{x,y} > 0$ for each $(x,y) \in E$. Let σ be any assignment of $\{0,1\}$ to each of the vertices. Then we define the *Hamiltonian* of σ as

$$H(\sigma) = \sum_{(x,y)\in E} J_{x,y} \mathbf{1}_{\sigma_x \neq \sigma_y},$$

where $\mathbf{1}_A$ is the indicator function which is 1 when the event A is true and 0 otherwise. The probability $\pi(\sigma)$ that the Ising spin state takes the value σ is given by the *Gibbs measure*:

$$\pi(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z(G)},$$

where β is inverse temperature and

$$Z(G) = \sum_{\sigma} e^{-\beta H(\sigma)} \tag{1}$$

is the normalizing constant referred to as the *partition function*. The partition function (1) has two other standard representations which we require, in particular, the Fortuin-Kasteleyn *random cluster* representation (2) and the *high temperature expansion* (3). Given a graph $G = (V,E)$, in both cases the state space now consists of subgraphs $\omega \subset E$ (or $G_\omega = (V,\omega)$). Define $p_{x,y} = 1 - e^{-\beta J_{x,y}}$. The partition function $Z(G)$ defined over spin configurations σ can be rewritten as

$$Z(G) = \sum_{\omega \subseteq E} \prod_{(x,y)\in\omega} p_{x,y} \prod_{(x,y)\in\omega^c} (1-p_{x,y})\, 2^{\#\omega}, \tag{2}$$

and as

$$Z(G) = \sum_{\omega\in \mathrm{Even}(E)} \prod_{(x,y)\in\omega} \frac{p_{x,y}}{2} \prod_{(x,y)\in\omega^c} \left(1-\frac{p_{x,y}}{2}\right) 2^n, \tag{3}$$

where $\#\omega$ is the number of components in ω and $\mathrm{Even}(E)$ is the set of subsets of E such that all of the vertices have even degree. Notice that in both cases $Z(G)$ is the expected value of a certain quantity when each edge occurs independently with probability $p_{x,y}$ (in the FK representation (2)) or $p_{x,y}/2$ (in the high temperature expansion (3)). As with spin configurations, we define the probability of a subgraph to be its contribution to $Z(G)$ in the above sums divided by $Z(G)$.

The Ising model allows physicists to study magnetization on a microscopic level, and many of the thermodynamic properties of an Ising system can be estimated from the partition function or from sampling typical spin configurations according to their Gibbs measure.

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Many heuristics involve clever sampling algorithms to study these properties. The celebrated Swendsen-Wang algorithm [11] which uses both the *spin* and the *random cluster* representation seems to be very efficient and is used extensively in practice, but typically results are not rigorous. Only recently has there been rigorous analysis of the Swendsen-Wang algorithm in special cases, and this is mostly in the form of negative results [6, 3] and in particular classes of graphs there are finally some positive results [3, 7].

A major contribution to the theoretical treatment of designing efficient and rigorous algorithms for studying quantities pertaining to an Ising system was due to Jerrum and Sinclair who developed an *fpras* (fully polynomial randomized approximation scheme) for approximating the partition function [8]. The analysis is based on their seminal work for rigorously bounding the conductance of a Markov chain and on the third representation of the partition function, the *high energy expansion*. Surprisingly, however, this did not lead immediately to a rigorous method for sampling spin configurations. While most natural problems are *self-reducible* and the framework formalized by Jerrum, Valiant, and Vazirani [9] provides reductions between approximate counting and random sampling, the high energy expansion does not admit a straightforward self-reduction by successively fixing the spins on some of the sites as one might expect. In addition to the physical applications for studying magnetization, algorithms which rely on sampling Ising configurations according to their Gibbs measure have been used in vision where it is not sufficient to approximate the partition function (see, e.g., [5, 1]).

In this note we present an *fully-polynomial approximate generator* for sampling spin configurations of any ferromagnetic Ising system; the algorithm outputs configurations σ with probability $P(\sigma)$ where $\pi(\sigma)/(1+\epsilon) \leq P(\sigma) \leq \pi(\sigma)(1+\epsilon)$ and it runs in time polynomial in n and $\log(1/\epsilon)$, where n is the size of the input graph.

The key observation is that the random cluster model is self-reducible. It is straightforward to verify that for any edge $\hat{e} \in E$,

$$Z(G) = p_{\hat{e}} Z(G^+) + (1 - p_{\hat{e}}) Z(G^-),$$

where G^+ is the graph formed by contracting the edge $\hat{e}$ in G and G^- is the graph formed by removing the edge $\hat{e}$. Using standard ideas and making successive calls to the Jerrum-Sinclair algorithm for approximating the partition function Z we get a generator for random cluster states $\omega \subset E$ according to the correct distribution.

To complete the algorithm we simply assign spins to each of the vertices so that all vertices within the same connected component of ω are assigned the same spin. The probability of each spin configuration occurs with precisely the probability defined by the Gibbs distribution, as demonstrated by Fortuin and Kasteleyn [4].

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