Theory and Methods for the Ferromagnetic Ising Model

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Abstract

The Ising model is a historically important problem in statistical mechanics. Although it was originally proposed as a crude approximation of ferromagnetic phenomena, it furnished statistical mechanics, and later probabilistic science as whole, with a new paradigm of graph-based modeling that would prove influential. Especially in the distilled, theoretical study of probabilistic graphical models (PGMs), which today is its own field, many methods developed for Ising models and spin-glasses have been repurposed and reinterpreted, as have the rich physical vocabulary of energies, entropy, and partition functions.

In this paper, we pay homage to the Ising model by applying modern methods to the original problem of ferromagnetism. We discuss the theory of the Ising model both from a PGMs and statistical mechanics point of view, examining the correspondence. We then evaluate two approaches to inference—Markov Chain Monte Carlo and belief propagation. Finally, we show the successes and limitations of the Ising model in the context of physical phenomena.

1 Theory of the Ising Model

The prevailing physical theory explains magnetism as a consequence of the intrinsic spin of particles. This spin produces a magnetic dipole moment $\vec{\mu}$ proportional to the spin σ:

$$\vec{\mu} = \mu\sigma$$

If an external magnetic field $\vec{B}$ is present, the potential energy is given by the classical formula:

$$U_B = -\vec{\mu} \cdot \vec{B}$$

Handily, this also absorbs the splitting of atomic energy levels due to quantum mechanical phenomena.

There also exists a pairwise interaction between particles due to the mutual effects of their magnetic moments. These exchange effects have strength defined by constants J_{ij}, The potential energy of these pairwise interactions is then:

$$U_{ij} = -J_{ij}\vec{\mu_i} \cdot \vec{\mu_j}$$

Here, we ignore quantum mechanical spin-spin coupling and exclusion energies.

Note that both potential energies are minimized when the moments align with $\vec{B}$ and with each other. This corresponds to the theory of ferromagnetism as a systematic alignment of spins.

Now, consider a collection of particles $\vec{\mu_i}$ in the prescence of an external magnetic field $\vec{B}$. The Hamiltonian, which specifies the total energy of the system, is defined by the sum of all pairwise and

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unary energies:

$$E(\vec{\mu}) = -\frac{1}{2}\sum_i \sum_j J_{ij}\vec{\mu_i}\cdot\vec{\mu_j} - \sum_i \vec{\mu_i}\cdot\vec{B} \tag{1}$$

In most cases, working with this Hamiltonian is intractable. Luckily, we can simplify it by making several strategic assumptions.

First, in the context of an atomic lattice, all relevant particles are fermionic and have spin-$\frac{1}{2}$. We assume that all particles within an atom have identical spin, so the spin of each atom as a whole is fermionic. Then the magnetic moments simplify to $\vec{\mu_i} = \mu\sigma_i$, where $\sigma_i \in \{-1, 1\}$ is the atomic spin.

Second, we make a mean-field nearest-neighbor approximation so that the strength of pairwise interactions are negligible for non-adjacent pairs. We also assume all non-negligible J_{ij}'s are equivalent, that is that the material is organized in a regular lattice.

Coalescing constants, the Hamiltonian reduces nicely to:

$$E(\vec{\sigma}) = -J\sum_i \sum_{j\in adj(i)} \sigma_i\sigma_j - \sum_i \sigma_i B_i \tag{2}$$

The Boltzmann distribution give a probability of some state $\vec{\sigma}$ at inverse temperature β:

$$P(\vec{\sigma}) = \frac{1}{Z}e^{-\beta E(\vec{\sigma})} \tag{3}$$

The physical theory of the Ising model has now been developed and we can turn to inference as a pure PGMs task.

2 Inference on Ising Models

In many cases, the Ising model of ferromagnetism is used to produce physical measurables like energy and magnetization. For example, Ernst Ising's original inquiry asked if the Ising model was capable of demonstrating phase transitions—changes in the magnetic state due to external conditions.

Now, these measurables require marginal distributions in order to compute, for example, the unary and pairwise energies. We will now examine two approaches to computing these marginals—Markov Chain Monte Carlo and belief propagation.

2.1 Markov Chain Monte Carlo

Monte Carlo algorithms produce better and better estimates by repeated sampling from the true distribution. When the true distribution is not immediately available for sampling, employing Markov Chain Monte Carlo defines an approximate distribution that hopefully, during sampling, approaching the true distribution.

In the context of the Ising model, the Markov states proceeding from some state of spins $\vec{\sigma}$ are created by flipping any spin σ_i in $\vec{\sigma}$. We can sample from these states by choosing a random σ_i to flip. Since we want to move towards the true, equilibrium distribution, we only transition to the new state $\vec{\sigma}'$ if $P(\vec{\sigma}') > P(\vec{\sigma})$. Using the formula for the Boltzmann distribution, this criterion is equivalent to $E(\vec{\sigma}') < E(\vec{\sigma})$.

In practice, we will compute the change in energy $\Delta E = E(\vec{\sigma}') - E(\vec{\sigma})$, which has a nice form:

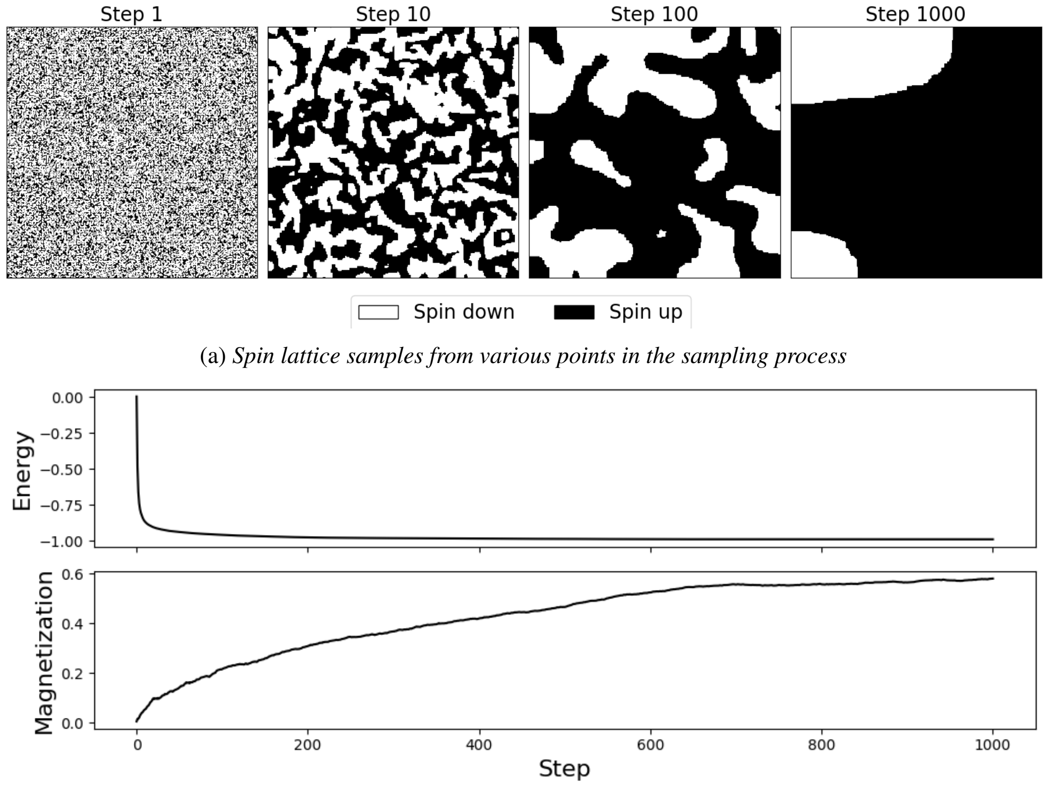
$$\Delta E = E(\vec{\sigma}') - E(\vec{\sigma}) = 2\sigma_i(J\sum_{j\in adj(i)}\sigma_j + B_i)$$

If $\Delta E < 0$, we transition states. If $\Delta E \geq 0$, we will transition states with probability defined by the Boltzmann factor:

$$\frac{P(\vec{\sigma}')}{P(\vec{\sigma})} = e^{-\beta\Delta E}$$

This nicely models the phenomena of spin flips caused by field fluctuations.

We implemented this process in Python on square lattices of spins. For our sampling process, we iterated through all spins in random order, at each step evaluating the transition defined by flipping the present spin. We believe this best simulates the actual equilibration process.



(a) *Spin lattice samples from various points in the sampling process*

(b) *Measurables of samples during the sampling process*

Figure 1: *MCMC quenching of an initial randomly generated* 256×256 *spin lattice sample with* $J = 0.5$*,* $\beta = 10$*, and a centered Gaussian magnetic field* $B_{ij} = 0.01 \exp[-\frac{1}{1024}((i-128)^2+(j-128)^2)]$.

In the MCMC quenching simulation conducted in 1, we observe several expected phenomena. The pairwise interactions are clearly exhibited by the clusters of aligned spins which form and coalesce as the number of steps grows. The prescence of the magnetic field also seems to magnetize the entire lattice, as indicated both by the convergence on full spin alignment in 1a, and the increasing magnetization measured in 1b.

Note that computing the measurables for 1a and 1b is easy given the explicit spin lattice states provided by the sampling process. The magnetization is simply the average spin. The energy is computed using 2. We will see that these measurables are not so easily obtained when using belief propagation.

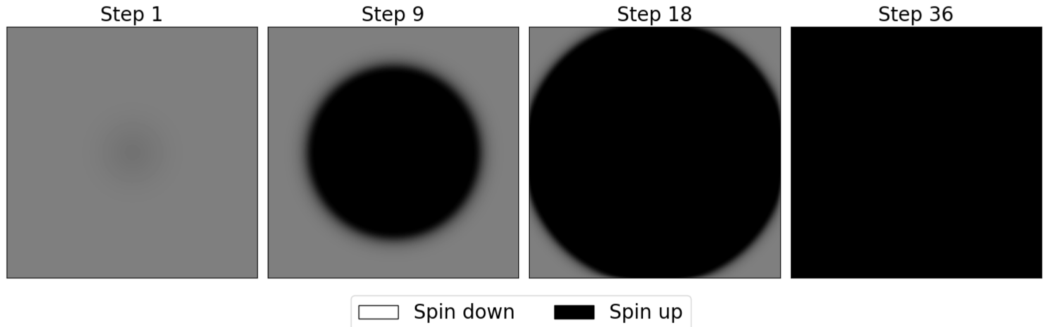
Plots describing additional simulations are shown in the Supporting Materials.

2.2 Belief Propagation

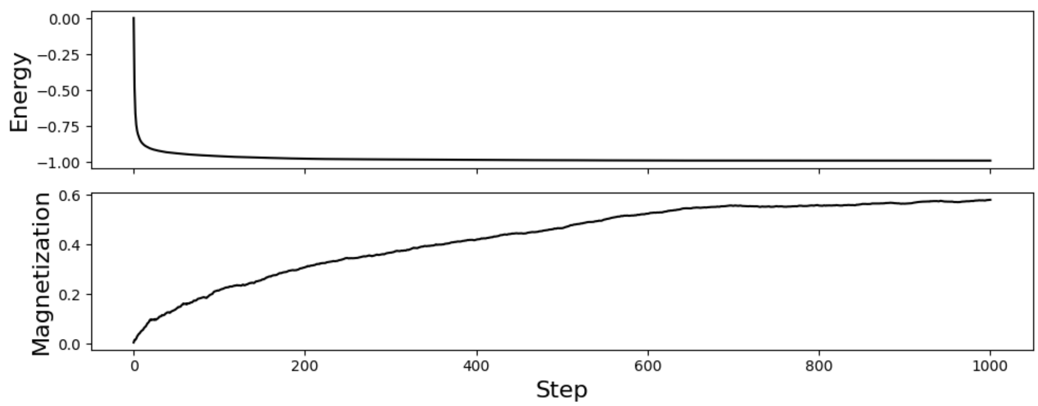
Message-passing belief propagation algorithms are another way to estimate true marginals for general graphical models. They are derived from the theory of variable elimination, but are applicable to general graphs which may include cycles.

It turns out that belief propagation is especially effective and simple to implement on Ising models. This follows from the Boltzmann distribution that defines the joint distribution of the Ising model:

$$\tilde{P}(\vec{\sigma}) = \exp\Big[\beta J \sum_{i} \sum_{j \in adj(i)} \sigma_i \sigma_j + \beta \sum_{i} \sigma_i B_i\Big] \tag{4}$$



(a) *Spin lattice beliefs from various steps in the belief propagation process*



(b) *Measurables of samples during the sampling process*

Figure 2: *Belief propagation to estimate marginal distributions of spin lattice with* $J = 0.5$, $\beta = 10$, *and a centered Gaussian magnetic field* $B_{ij} = 0.01 \exp[-\frac{1}{1024}((i-128)^2 + (j-128)^2)]$.

It factorizes nicely over the Ising lattice:

$$\tilde{P}(\vec{\sigma}) = \prod_i \exp\Big[\beta \sigma_i B_i\Big] \prod_{j \in adj(i)} \exp\Big[\beta J \sigma_i \sigma_j\Big] \tag{5}$$

This defines a factor graph of node and edge potentials representing the unary and pairwise potentials, respectively:

$$\phi_i = \exp\Big[\beta \sigma_i B_i\Big] \qquad\qquad \phi_{ij} = \exp\Big[\beta J \sigma_i \sigma_j\Big]$$

We then run a standard belief propagation routine.