
Phase Transition of Ising Model with Belief Propagation

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Abstract

Ising models have traditionally been solved with Markov chain Monte Carlo methods, the most popular of which is the Gibbs' sampler. However, MCMC suffers from correlated samples and long mixing times. In recent years, a new class of algorithms based on variational inference has come to light. These algorithms promise faster convergence at the cost of convergence. Belief propagation is an inference algorithm that uses message passing in order to approximate the probability distribution over a factor graph. In this paper, we apply belief propagation to solve the Ising model and show that during belief propagation, the 2D Ising model exhibits a phase transition similar to simulations using MCMC. We compare metrics of phase transitions to MCMC approaches and known theoretical results and conclude that belief propagation can solve the Ising model to a high degree of accuracy and retain many interesting properties that the Ising model is known for.

1. Introduction

The Ising model is a mathematical model of ferromagnetism in statistical mechanics. Invented first by Wilhelm Lenz in 1920 and the equations of the one-dimensional Ising model were solved in by Lenz's student Ernst Ising in 1924. In 1944, Lars Onsager solved the equations for the two-dimensional case. As of today, no analytic solution has been found in dimensions three or higher. Over the last 100 years, many other problems such as percolation, min cut max flow, error correction, neural networks, and neurodegenerative diseases were shown to be very closely mathematically related to the Ising model. The Ising model's relatively simple formulation yet rich and general mathematical properties makes a *drosophila* of physics, mathematics, statistics, and computer science.

Since Onsager's solution, it is known that the Ising model

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exhibits a phase transition just like magnets in the real world. Above the a special temperature, the critical temperature (or more generally the critical point), the system under goes a rapid change, changing from an ordered magnetic state to a disordered non-magnetic state. This rapid change of order is fundamentally related to the relationship between energy, entropy and free energy. When the system is at the critical point, it is said to be at criticality and many interesting properties such as scale invariance and long range correlations are present during the phase transition.

However, due to the difficulty of solving the Ising models in higher dimensions, many approximation methods have been devolved over the years. Statistical physicists developed mean field theory and the cavity method to find approximate analytic solutions. In more recent times, the rise of computational power allowed computer algorithms to approximate solutions to the Ising model. The most well known class of algorithms are Markov Chain Monte Carlo (MCMC) algorithms such as Metropolis-Hasting algorithm and Gibbs' sampling. Although these algorithms are powerful and still widely used, they suffer long convergence times and autocorrelated samples.

In this paper, we explore an alternative algorithm to approximately solve the Ising model called belief propagation. Belief propagation works by sending messages from each node of a factor graph to iteratively find the probability distribution. We show that this method can calculate solutions comparable to Metropolis-Hastings and Gibbs sampling and show that solutions given by belief propagation exhibit a phase transition like predicted theoretically.

2. Background

2.1. Ising Model

The Ising model models ferromagnetic materials as a two-dimensional lattice where each lattice site represents an electron that is either spin up $\sigma_i = +1$ or spin down $\sigma_i = -1$. Each lattice point only interacts with its adjacent neighbors. In this paper, we impose periodic boundary conditions. This is equivalent to the lattice wrapped around the surface of a torus. This simulates an infinitely large lattice and mitigates boundary effects. Thus, the total energy (also known as the

Hamiltonian H in physics literature) is

$$E(\sigma) = -J \sum_{(i,j) \in \mathcal{N}} \sigma_i \sigma_j - B \sum_j \sigma_j \quad (1)$$

where $(i, j) \in \mathcal{N}$ is understood to be the sum over all pairs of (i, j) that are adjacent neighbors, J is the physical constant known as the coupling strength and B is the strength of the external magnetic field. We assume $J = 1$ for simplicity and no external magnetic field $B = 0$. Then our total energy is

$$E(\sigma) = - \sum_{(i,j) \in \mathcal{N}} \sigma_i \sigma_j \quad (2)$$

We notice that the energy is lower when σ_i and σ_j are the same sign and greater when σ_i and σ_j are different signs. The energy is minimized when the spins are aligned in the same direction, corresponding to a magnetized state. However, the entropy is maximized when the spins are misaligned corresponding to a demagnetized state.

The PMF of the system is given by the Boltzmann distribution

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

where the inverse temperature $\beta = 1/(kT)$, k is Boltzmann's constant, and the normalization constant $Z = \sum e^{-\beta H(\sigma)}$. Given an initial square lattice of σ and inverse temperature β the goal is to find the equilibrium distribution over σ .

2.2. Phase Transition

In physics a phase transition refers to a change of a system from one state to another. A classical example is ice melting into water. However, more generally it refers to the rapid change of a system's order parameter as a function of one or more of the system's parameters. This more general definition can be applied to other fields such as rate distortion theory. The Ising model predicts a phase transition of a ferromagnetic system like an iron magnet from a demagnetized state to a magnetized state. It is known empirically that heating a magnet above a certain temperature known as the Curie temperature (770 °C for iron) causes rapid demagnetization. The characteristic feature of the phase transition is that the magnetization strength changes very rapidly over a short range of temperature similar to how ice melts into water over a narrow temperature range of 0°C. This transition from order to disorder is due to the changing strength of energetic and entropic forces.

In nature, systems tend to minimize a thermodynamic quantity known as free energy. The free energy is given by

$$F = E - TS \quad (4)$$

where S is the thermodynamic entropy. At high temperatures the entropy term is dominant and at low temperature the energetic term is dominant. This explains why the spins are misaligned at high temperature. The thermal energy from the environment is sufficient to flip the lattice site spins. This thermal function acts like a corrupting force constantly disrupting the spins of the system. It is also convenient to define the free energy as

$$F = kT \ln Z \quad (5)$$

The normalization constant Z is called the partition function and it turns out it is very important. These two formulas are equivalent

$$S = -k \sum_i p_i \ln p_i \quad (6)$$

$$= -k \sum_i \frac{e^{-\beta E_i}}{Z} \ln \left(\frac{e^{-\beta E_i}}{Z} \right) \quad (7)$$

$$= -k \sum_i \frac{e^{-\beta E_i}}{Z} (-\beta E_i - \ln Z) \quad (8)$$

$$= k\beta \sum_i \frac{e^{-\beta E_i}}{Z} E_i + k \sum_i \frac{e^{-\beta E_i}}{Z} \ln Z \quad (9)$$

$$= k\beta \langle E \rangle + k \ln Z \quad (10)$$

$$= k\beta E + k \ln Z \quad (11)$$

since the energy E is simply the energy averaged all over microstates $\langle E \rangle$. Plugging this into (4) yields

$$F = E - T(k\beta E + k \ln Z) \quad (12)$$

$$= E - T \left(k \frac{1}{kT} E + k \ln Z \right) \quad (13)$$

$$= E - E + kT \ln Z \quad (14)$$

$$= kT \ln Z \quad (15)$$

The energy can also be defined in terms of the partition function as

$$E = -\frac{\partial \ln Z}{\partial \beta} \quad (16)$$

$$= -\frac{1}{Z} \frac{\partial Z}{\partial \beta} \quad (17)$$

$$= -\frac{1}{Z} \frac{\partial}{\partial \beta} \sum_i e^{-\beta E_i} \quad (18)$$

$$= -\frac{1}{Z} \sum_i -E_i e^{-\beta E_i} \quad (19)$$

$$= \sum_i E_i \frac{e^{-\beta E_i}}{Z} \quad (20)$$

$$= \langle E \rangle \quad (21)$$

$$= E \quad (22)$$

These equations will be relevant when we discuss the connection between belief propagation and minimization of the Bethe free energy.

By analyzing at what temperature the energy and entropy terms balance, Onsager solved the 2D Ising model analytically in the case of no external magnetic field and showed that the critical temperature is

$$T_c = \frac{2J}{k \ln(1 + \sqrt{2})} \quad (23)$$

or in terms of $\beta_c = \frac{\ln(1+\sqrt{2})}{2J}$. This derivation is very technical and will not be covered here.

The Ising model at the critical temperature exhibits many interesting properties. The first is the rapid change of the order parameter, in the case of the Ising model, the magnetization given the average value of the spins.

$$\langle M \rangle = \frac{1}{N} \sum_{i=1}^N \sigma_i \quad (24)$$

In order to not give preference to major spin down or spin up configurations, it is convenient to define the magnetization squared $\langle M^2 \rangle = \frac{1}{N} \sum_{i=1}^N \sigma_i^2$.

At the critical temperature, the system reaches a critical state where order and disorder are perfectly matched. Here, the model exhibits long range correlations not found at other temperature regimes. The Ising model only takes into account interactions between neighboring lattice sites. Therefore, we expect the correlation between lattice sites to be very short and lattice sites long distances apart to act independently. This is in general true except when the system is at criticality. When order and disorder are perfectly balanced, local interactions have a ripple effect, meaning that

local interactions lead to long range communication. The correlation function is given by

$$C_{i,j} = \langle (\sigma_i - \langle \sigma_i \rangle)(\sigma_j - \langle \sigma_j \rangle) \rangle \quad (25)$$

where the $\langle \cdot \rangle$ denotes the time average.

Then we can define the correlation length function,

$$C(d) = \mathbb{E}[C_{i,j} \mid D(i,j) = d] \quad (26)$$

Another interesting phenomena observed at criticality is scale invariance. Suppose for each 3 by 3 block of spins, we replace that block with the spin corresponding to the majority spin value out of those 9 smaller spins. Apply this procedure to the whole lattice and we have a new lattice with a third of the distance scale. This procedure is called a course graining. We can continue this procedure indefinitely on an infinitely large lattice. At the critical point, all these lattices of varying length scales look the same, in other words there is no characteristic scale. To show this idea graphically, we plot the distribution of the cluster sizes where a cluster is a group of lattice points with the same spin. If the distribution of the cluster sizes is scale invariant, they should follow a power law

$$f(x) = Ax^{-\gamma} \quad (27)$$

where $f(x)$ is the probability of observing a cluster size with size x . We can visualize this as a straight line on a log-log plot where the slope is γ .

3. Methods

3.1. Metropolis-Hasting

3.2. Gibbs Sampler

3.3. Belief Propagation

4. Experiments

5. Discussion

6. Conclusion