Theory and Methods for the Ferromagnetic Ising Model

TTIC 31180

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5/21/2024

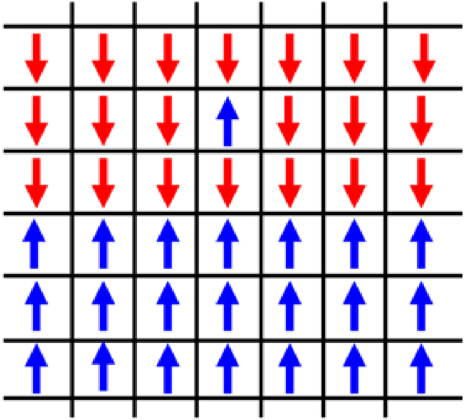
Outline

1. Review of the Ising Model

2. Inference Using the Ising Model

Review of the Ising Model

What is an Ising Model?



- The Ising model is used in statistical mechanics to describe ferromagnetism in materials.
- Each site on the lattice is associated with a spin, which represents the magnetic moment of an atom or molecule.
- The spins are subject to thermal fluctuations, causing them to flip between $\{-1,1\}$.

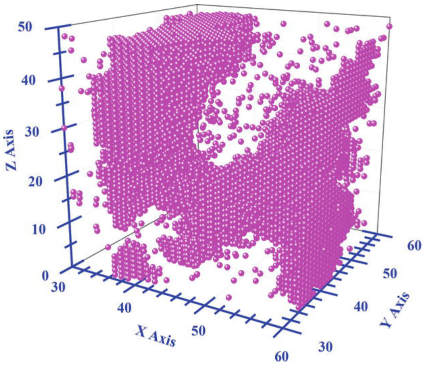
Theory of the Ising Model

- A particle with magnetic moment $\vec{\mu}$ in an external magnetic field $\vec{B}$ has potential energy:

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

- The magnetic moment also creates a magnetic field. The interaction between particles, denoted by exchange constants J_{ij}, also have potential energy:

$$U = -J_{ij}\vec{\mu_1} \cdot \vec{\mu_2}$$



Theory of the Ising Model cont.

- So now we have a collection of particles in the presence of an external magnetic field. The Hamiltonian, which specifies the total energy of the system, is defined by the sum of all pairwise and all magnetic field energies:

$$E = -\frac{1}{2}\sum_{i,j} J_{ij}\vec{\mu_i}\cdot\vec{\mu_j} - \sum_i \vec{\mu_i}\cdot\vec{B}$$

- This is intractable, and we can simplify it through several assumptions. By coalescing constants,

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

Theory of the Ising Model cont.

- Following the Boltzmann distribution, the probability of some state $\vec{\sigma}$ at inverse temperature β is:

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

Inference Using the Ising Model

Inference Using the Ising Model

- The motivation to perform inference on the ising model is to find the equilibrium distribution of spins that minimize the energy
- In our project, we tested two commonly used methods: MCMC and Belief Propagation.

Markov Chain Monte Carlo (MCMC)

- Sampling from the conditioned distribution corresponds to flipping some spins of some spin state $\vec{\sigma}$ to get a new spin state $\vec{\sigma}'$. If the new spin state is more probable than the previous one, then we flip to the new state. We write the transition "probability" as:

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

- In the case where only one spin σ_i flips, we can write the energy difference in the exponential as $E(\vec{\sigma}') - E(\vec{\sigma}) = 2\sigma_i(J \sum_{j \in adj(i)} \sigma_j + B_i)$

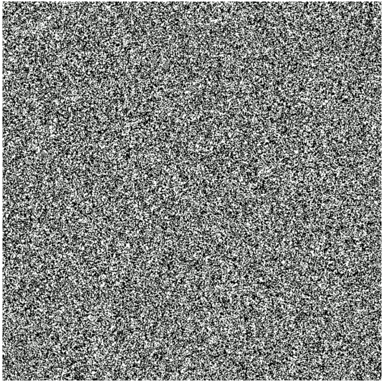
Markov Chain Monte Carlo (MCMC) cont.

- The final expression is therefore:

$$P_{\vec{\sigma}\to\vec{\sigma}'} = exp(-2\beta\sigma_i(J\sum_{j\in adj(i)}\sigma_j + B_i)))$$

- If the transition lowers the energy, accept it. Otherwise, accept it with probability $P_{\vec{\sigma}\to\vec{\sigma}'}$

Results of MCMC cont.



Belief Propagation

The joint distribution of the Ising model is:

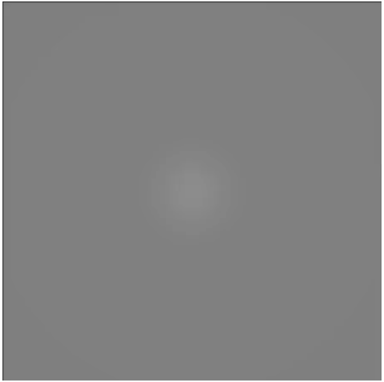
$$P(\vec{\sigma}) = \exp\left[\beta\left(J\sum_{i}\sum_{j\in adj(i)}\sigma_i\sigma_j + \sum_{i}\sigma_i B_i\right)\right]$$

This factors nicely as:

$$P(\vec{\sigma}) = \prod_{i}\prod_{j\in adj(i)}\exp(J\beta\sigma_i\sigma_j)\cdot\prod_{i}\exp(\sigma_i\beta B_i)$$

We can then define a factor graph of unary and pairwise potentials and use belief propagation for inference.

Belief Propagation cont.

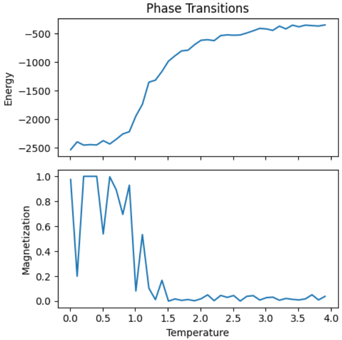


Sample-Based vs Belief Propagation

- Sample based inference has a hard time converging.
- Belief propagation gives a distribution while MCMC gives a set of samples.
- MCMC is more physically intuitive.

Discussion

- We simulate some phase transitions using MCMC:



Thank You

Questions?