Simulating Ising Model

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Agenda

1. Background Information
   1. Ising Model, Onsager exact solutions, Monte Carlo Markov Chain
2. Algorithm
3. Simple Ising Model
4. Ising Model with external magnetic field
   1. scalar field, vectorized field
5. Simulation

Ising Model

- Developed by Ernst Ising
- Simplified version of Ferromagnets
- Phase transition

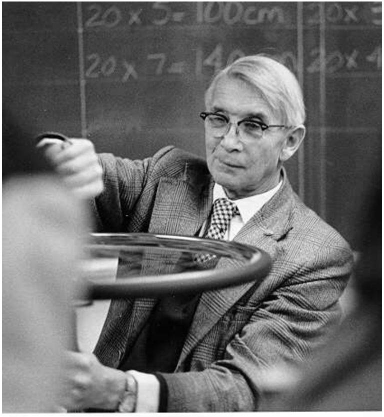


Figure: Enrst Ising

Ising Model

- Represented by a lattice grid
- Each lattice site contains a single magnetic moment of atomic spins
- We represent each spin as +1 (spin up) or -1 (spin down)

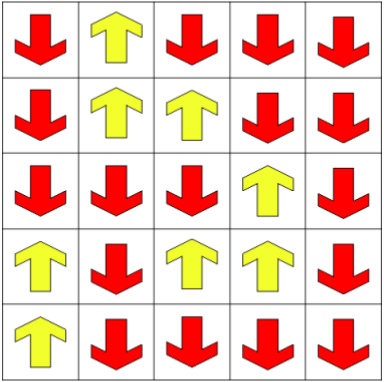


Figure: Sample lattice

Ising Model

- When all lattice site spins align, we see a net magnetic in the macroscopic scale
- The Hamiltonian of the site j is

$$H_j = -J \sum_{<ij>} S_i S_j - k \sum_j S_j$$

where J is the coupling interaction with its neighbors, notation $\sum_{<ij>} S_i S_j$ is the sum of the neighbors around S_j, and k is the external magnetic field.

Ising Model - Observable Quantities

- The magnetization M can be found as

$$M = \frac{1}{N} \sum_{i=1}^{N} S_i$$

- The total energy E can be found as

$$E = \sum_{i=1}^{N} H_j$$

$$E = \sum_{i=1}^{N} (-J \sum_{<ij>} S_i S_j - k \sum_{j} S_j)$$

Ising Model - Observable Quantities

- Magnetic Suspectibility, X can be found as

$$X = \left(\frac{1}{N}\sum_{i=1}^{N} S_i^2\right) - M^2$$

- Specific Heat, C can be found as

$$C = \left(\sum_{i=1}^{N} H_j^2\right) - E^2$$

Onsager Exact Solutions

- Onsager's exact solution for critical temperature is

$$\sinh\left(\frac{2J_1}{kT_c}\right)\sinh\left(\frac{2J_2}{kT_c}\right) = 1$$

  where J_1 and J_2 is the horizontal and vertical coupling interactions between the neighbor atoms, k is the boltzmann constant, and T_c is the critical temperature.

- For simplicity, $J_1 = J_2 = J$, we can find the temperature where the phase transition happened as

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

Onsager Exact Solutions

- Onsager's exact solution for magnetization is

$$M = \left(1 - [\sinh(2\beta J_1)\sinh(2\beta J_2)]^{-2}\right)^{\frac{1}{8}}$$

where $\beta = \frac{1}{T}$.

- For simplicity, $J_1 = J_2 = J$, the equation becomes

$$M = \left(1 - [\sinh(2\beta J)]^{-4}\right)^{\frac{1}{8}}$$

for $T < T_c$ and 0 for $T > T_c$, where $\beta = \frac{1}{T}$.

Monte Carlo and Markov Chain

- Monte Carlo is a randomized algorithm that is to approximate certain behaviors
- Markov Chain is an algorithm that will move into a state with high probabilities. It is dependent on the previous state.

Algorithm

1. Create a 2D lattice of size NxN.
2. Fill the lattice $+1$ and -1 randomly
3. Randomly select a site on the lattice
4. Flip the spin on the randomly selected site
    1. Calculate the change in energy,ΔE, when we flip the spin
5. **If** $\Delta E \leq 0$:
    1. Then we want to flip the spin
6. **Else** $(\Delta E > 0)$:
    1. Calculate the Boltzmann probability p,
    $$p = e^{-\beta \Delta E}$$
    2. Generate a random number u between 0 and 1.
    3. **If** $u \leq p$ then we want to flip the spin
    4. **Else** Revert back to the original spin
7. Repeat steps $3 - 6$ until convergence

Let's consider Ising model where external magnetic field is 0

Figure: Initial Lattice $N=50$

Simple Ising Model (Temp << Critical Temp)

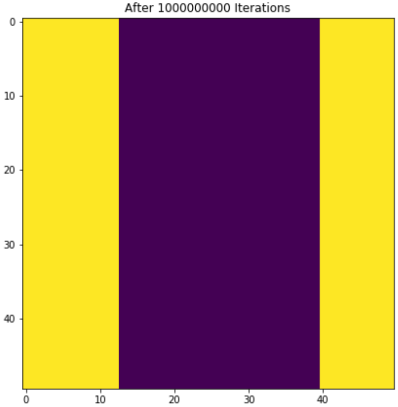


Figure: MCMC simulation with $J = 2$ and Temperature $= 0.001$ K

Simple Ising Model (Temp >> Critical Temp)

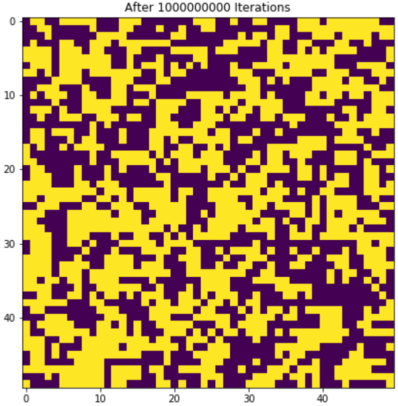


Figure: MCMC simulation with $J = 2$ and $T = 5$ K

Simple Ising Model ($J < 0$; Temp $<<$ Critical Temp)

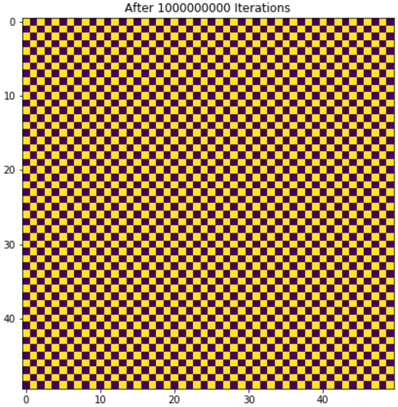


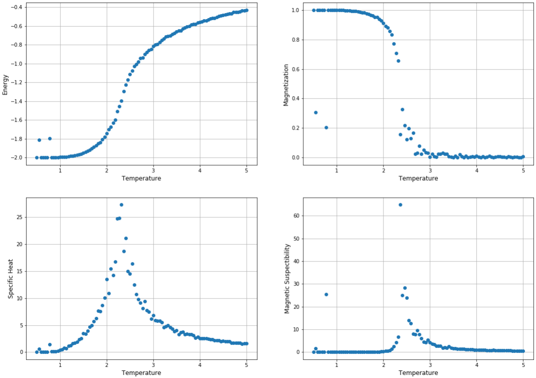
Figure: MCMC simulation with $J = -2$ and $T = 0.005$ K

Simple Ising Model ($J < 0$; Temp $>$ Critical Temp)

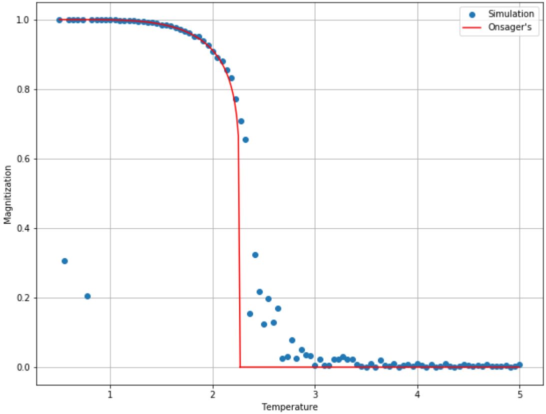
Figure: MCMC simulation with $J = -2$ and $T = 3$ K

Observable Quantities

In this section we will calculate the observable quantities from our simulation.
Using $N = 22$, $J = 2$ for simulation:



Comparison to Onsager's exact solution



Ising Model with External Field

Let's consider an Ising Model when external magnetic field $k \neq 0$. Applying scalar magnetic field on the all the atoms in the site.

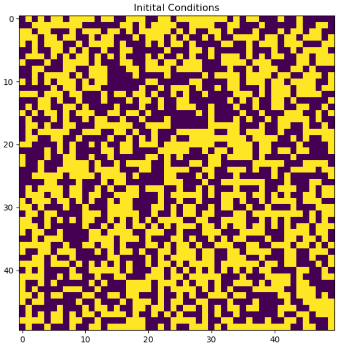


Figure: Initial lattice conditions

Ising Model with Scalar External Field

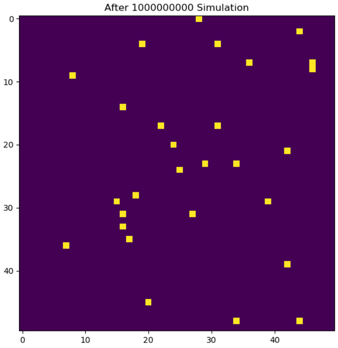


Figure: MCMC simulation with $J = 2$, $T = 3$ K, $k = 6$

Ising Model with Vectorized External Field

Often times, magnetic field comes in as vector field
Let's apply a simple vector field on our model.

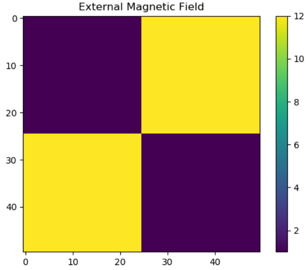


Figure: Magnetic Field

Ising Model with Vectorized External Field

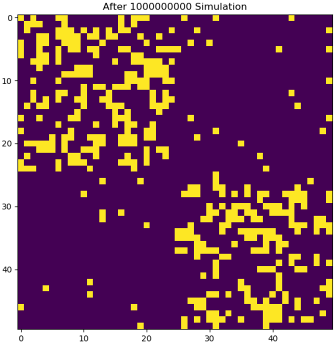


Figure: MCMC simulation $T = 4$, $J = 2$

Simulation