Computer Simulation of Ising Model

Shubham Raghubanshi
Anirban Bhattacharjee
Shouvik Bhattacharjee
Sawani Datta

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1 Introduction

Ising Model is a mathematical model of feromagnetism and simulate the structure of feromagnetic substance. In this model,the system considered is an arrary of N fixed lattice sites. A spin variable σ_i (i=1,2,...,N) is associated with each lattice site,it can take value either +1 or -1. This model predicts a 2^{nd} order phase transition occuring at the Curie temparature for dimension greater than 1.

2 Definition

A set of lattice sites L,each with a set of adjacent sites forms a d-dimensional lattice and the lattice is modeled as periodic. Now for each lattice site K ϵ L, there is a discrete spin variable σ_k such that $\sigma_k \epsilon \{+1, -1\}$, representing the site's spin.

This model is defined in the **canonical ensemble** (N,V,T) and the Hamiltonian is defined as below.

$$H = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i$$

where

J_{ij} = coupling parameter between adjacent atoms,

h = external field strength.

We can simplify the model by assuming that all of the nearest neighbour have the same interaction strength si with such assumption we can can set the interaction parameter $J_{ij} = J$, $\forall(i,j)$

$$H = -J\sum_{<i,j>} \sigma_i\sigma_j - h\sum_i \sigma_i$$

Using this model, we can calculate the critical temperature for the phase transition

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

Using this model ,we can calculate specific heat and magnetisation by the following formulae,

$$C_v = \frac{(\Delta H)^2}{K_B T^2}, (\Delta H)^2 = \langle H^2\rangle - \langle H\rangle^2$$

and magnetisation per site is given by,

$$M = \frac{1}{L}\langle\sum_i \sigma_i\rangle = \frac{1}{L}\langle N_+ - N_-\rangle$$

3 Monte Carlo methods for numerical simulation

If there are many states in the system, the Ising model will be difficult to evaluate numerically. The **Metropolis-Hastings algorithm** is the most commonly used **Monte Carlo Algo -rithm** to calculate Ising model estimations. It is used for achieving an equilibrium energy.

3.1 Metropolis Algorithm

The algorithm first choose the **selection probabilities** $g(\mu,\nu)$ which represents the probability that state ν is selected by the algorithm out of all states ,given that we are in state μ. It then uses **acceptance probabilities** $A(\mu,\nu)$ so that **detailed balance** is satisfied. When implementing the algorithm we must ensure that $g(\mu,\nu)$ is selected such that **ergodicity** is met. Here we used the concept of **single-spin -flip dynamics** which states that in each transition we will only change one of the spin sites on the lattice.

Since there are L total sites on the lattice, using single-spin-dynamics, we can generate L new states ν from our present state μ. Here $g(\mu,\nu)=1/L$. From **detailed balance** we can say that:

$$\frac{A(\mu,\nu)}{A(\nu,\mu)} = \frac{g(\mu,\nu)A(\mu,\nu)}{g(\nu,\mu)A(\nu,\mu)} = \frac{A(\mu,\nu)}{A(\nu,\mu)} = \frac{P_\beta(\nu)}{P_\beta(\mu)} = \frac{\frac{1}{Z}e^{-\beta(H_\nu)}}{\frac{1}{Z}e^{-\beta(H_\mu)}}$$

$$= e^{-\beta(H_\nu - H_\mu)}$$

so the acceptance algorithm is:

$$A(\mu,\nu) = \{^{e^{-\beta(H_\nu-H_\mu)}, if(H_\nu-H_\mu)>0}_{1, otherwise}$$

• **Basic form of the algorithm:**

1. We picked a spin site using selection probability $g(\mu,\nu)$ and calculated the contribution to the energy involving this spin.

2.We then flipped the value of the spin and calculated the new contribution.

3.If the new energy is less we kept the flipped value.

4.But if the new energy is more we kept it with probability $e^{-\beta(H_\nu-H_\mu)}$.

5.The above mentioned steps were repeated until an equilibrium was reached.

3.2 Autocorrelation

Autocorrelation between two spin configuration is given by,

$$\rho(X,Y) = \frac{\sum_i^N (X_i - m)(Y_i - m)}{\sqrt{\sum_i^N (X_i - m)^2 \sum_j^N (X_j - m)^2}}$$

which falls exponentially with the number of iteration of Marcov Chain between two consecutive configuration is increased.

4 comparison with analytical results

4.1 Meanfield Approximation:

in mean field approximation, the qualitative nature of the critical behaviour can be obtained.The Weiss mean field theory gives

$$m = tanh(\beta h + \beta J z m)$$

where z is the coordination number and for 2D, z=4.

We can see that at low temp, there is a large value of the magnetisation and at higher temperatures, the value becomes zero.

4.2 Series expansion

4.2.1 Low Temperature Expansion:

At low temperatures, Z for Ising model with hamiltonian

$$-\beta H = K \sum_{<i,j>} \sigma_i \sigma_j$$

can be written as

$$Z = 2e^{2NK}[1 + Ne^{-8K} + 2Ne^{-12K} + \frac{N(N-3)}{2}e^{-16K} + ...]$$

$$\frac{C_v}{NK_B} = K^2[64e^{-8K} + 288e^{-12K} + 40e^{-16K} + ...]$$

where K=β J.

4.2.2 High Temperature Expansion:

Similarly for high temperature limit, the partition function is given by

$$Z(K) = (2cosh^2(K))^N[1 + N(tanh(K))^4 + 2N(tanh(K))^6 + ...]$$

Using these Z, we have calculated C_v in Mathematica.

4.3 Exact solution:

Using Onsager's exact solution for 2-D Ising model,we obtained the following thermodynamic quantities;The critical temparature is given by,

$$T_c = \frac{2J}{K_B ln(1+\sqrt{2})} = \frac{2.269J}{K_B}$$

magnetisation is given by,

$$m = \begin{cases} (1-(sinh(2\beta J)^{-4}))^{1/8} & ,for T<T_c \\ 0 & ,for T>T_c \end{cases}$$

and C_v is given by,

$$\frac{C}{K_B} = \frac{2}{\pi}(2\beta_c J)^2[-ln|1 - \frac{T}{T_c}| - ln(2\beta_c J) - (1 + \frac{\pi}{4})]$$

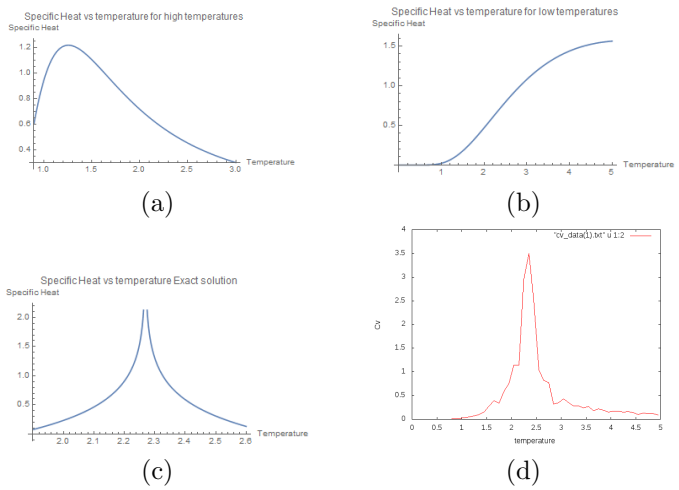

Figure 1: Fig.a shows Cv vs T plot for high temperature, Fig.b shows Cv vs T plot for low temperature, Fig.c shows Cv vs T plot for exact solution, Fig.d shows Cv vs T plot using our simulation.

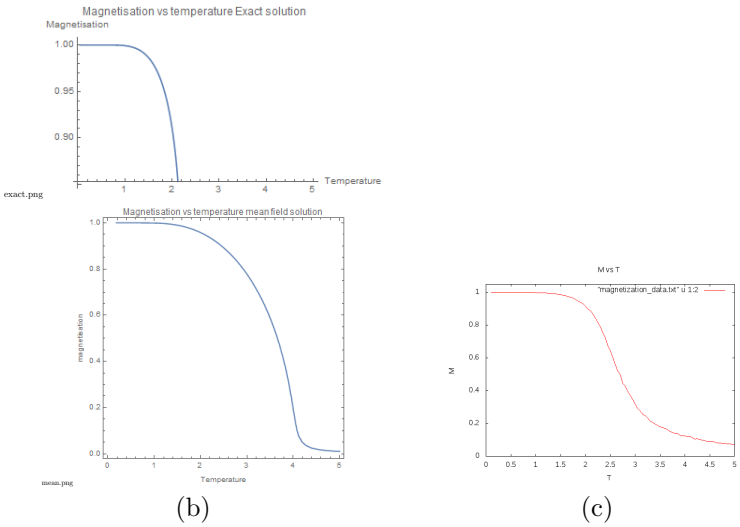

Figure 2: Fig.a shows m vs T for exact solution, Fig.b shows m vs T plot for mean field approximation, Fig.c shows m vs T plot using our simulation.

5 Conclusion

We have simulated the Ising model numerically using the Metropolis Algorithm and compared the plots with meanflied approximation ,series expansion and Onsager's exact solution.

Since it is a 2-D lattice of finite size, no phase transition was observed.

6 Acknowledgement

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References

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