PHSX815_Project4:
Monte Carlo Simulation of 2D Ising Model using Metropolis Algorithm

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1 Introduction

The Ising model has been used to explain a variety of phenomena in physics, chemistry, and other disciplines. It is particularly useful in studying the behavior of ferromagnetic materials, where the alignment of magnetic moments plays a crucial role. The Ising model was first introduced by Ernst Ising in 1925 [1] to study the behavior of magnetic moments in a lattice of spins.
This model depicts a ferromagnetic material as a lattice of discrete spins, each of which can represent an atom's magnetic moment by being either "up" or "down". The spins interact with each other through an energy term that depends on their relative orientation. In one dimension, with the spins organized in a line, the Ising model can be analytically solved and there is not a phase transition [1].In two dimensions the model exhibits a phase transition at a critical temperature known as the Curie temperature. Below the Curie temperature, the spins are aligned and the material has a net magnetization, while above the Curie temperature, the spins are randomly oriented and the material is non-magnetic. The model was analytically described by Lars Onsager in 1944 [2]. The analytic solution by Osanger gives enengy as follow:

$$H = -J \sum_{<i,j>} S_i S_j \tag{1}$$

The energy here represents the sum of all adjacent spin pairs, J is a constant that represents the strength of the interaction between neighboring spins, Si and Sj are the values of the spins at sites i and j in the lattice.
Also, the Specific Heat and the Magnetization are giving as the following:

$$C_v = \frac{< E^2 > - < E >^2}{T^2} \tag{2}$$

$$< M >=< \sum_i S_i > \tag{3}$$

While Onsager's solution predicts a phase transition at Tc= 2.269 J [3], the Ising model becomes much more complex with two dimensions and higher and it can be studied using computational methods such as Monte Carlo simulations. In this project, I will use Monte Carlo simulation for 2D Ising model and estimate the critical temperature at phase transition.

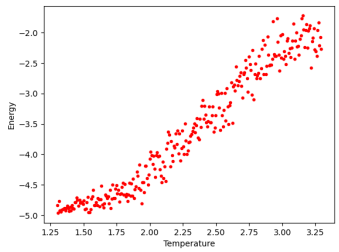
2 Code and Experimental Simulation

Let's look at some simulated data: First, I use Monte Carlo (Metropolis-Hastings algorithm) for 2D ising model [4] [5] as follow:
1/Prepare some random configuration of spins Si for each site in the lattice.
2/ Choose a random site i and calculate the change in energy (delta(E)) that would result from flipping the spin Si.
a) If delta E is less than zero, accept the flip and update the configuration.
b) If delta E is greater than zero, accept the flip with probability p = exp(-delta E/kT), where k is the Boltzmann constant and T is the temperature of the system.
3/Repeat the Metropolis-Hastings algorithm for a large number of steps to allow the system to equillibrate, and then sample the spin configurations to estimate the specific heat. To find the critical temperature, I fit a power function curve (with guess value of Tc) to data representing the specific heat as a function of temperature. Then, I use the (curvefit) function from Scipy.optimize [6] [7] to estimate the optimal value as critical temperature. In order to estimate the uncertainty in the critical temperature, I use a resampling technique (bootstrap) by resampling the original specific heat data with replacement. After that, I calculated the mean and standard deviation as uncertainty.
since the simulation run slowly as the algorithm updates each spin of the lattice once per Monte Carlo step, I use Numba to improves the speed of the simulation.

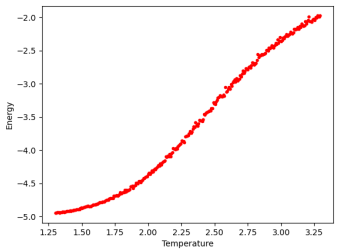
3 Analysis

The energy data as a function of temperature is depicted in Figure. 1. This figure shows how the energy values changes with change of the lattice size NXM and the number of Monte Carlo sweeps. For a small number of sweeps like 100, the data fluctuated and scattered.So, the system may not have enough time to explore a sufficient number of configurations and reach a stable state. On the other hand, as the sweep increases to 100000, the energy curve becomes smoother and more well-defined. Hence, the system has more opportunities to explore different configurations and reach a more stable state. The size of lattice affect the energy curve. For larger lattice sizes like 20X20, the curve seems similar to 5X5 with the same number of sweeps, but the simulation time increases. I could not do simulation for lattice with 20X20 with 1000000.

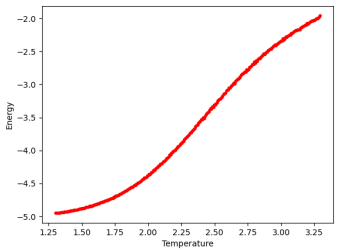
In order to determine the critical temperature, I calculated the specific heat as a function of temperature. Figure. 2. is showing the curve of specific heat at different value of temperatures including Tc. Similar to energy curve, with small weep number, the curves are not well-defined and scattered. Also, the curves seem smooth with high number of Monte Carlo steps.
The critical temperature value changes every time as I run the code, but it is close to the exact value. For example, the simulation of 5X5 lattice size and 10000 sweeps gives a Tc= 2.2698 with uncertainty of 0.0158. In the literature, the uncertainty was estimated using bootstrap method in 3D Ising model [8]. So, I calculated uncertainty in the critical temperature by performing bootstrap resampling by randomly sampling the specific heat data with replacement, fitting the power function to the bootstrap sample and extract best Tc value. Then, repeat N times to obtain a distribution of critical temperatures, from which the mean and standard deviation are calculated as uncertainty.



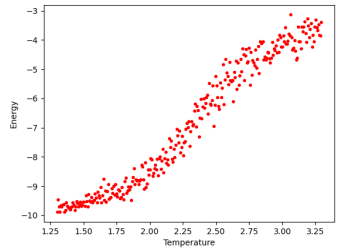
(a) lattice size 5X5 and sweep N= 100



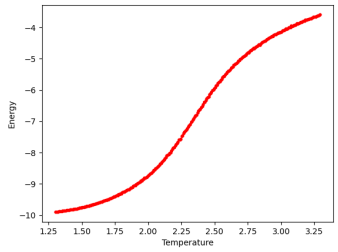
(b) lattice size 5X5 and sweep N= 10000



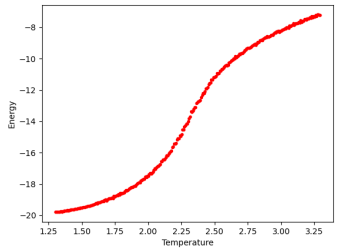
(c) lattice size 5X5 and sweep N= 100000



(d) lattice size 10X10 and sweep N= 100

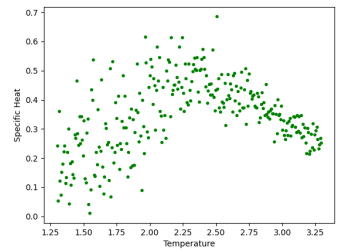


(e) lattice size 10X10 and sweep N= 10000

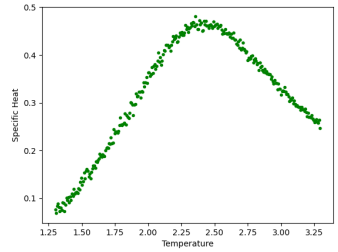


(f) lattice size 20X20 and sweep N= 10000

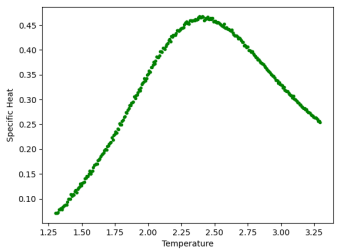
Figure 1: Plots of Energy as a function of Temperature for different lattice sizes and Monte carlo sweeps



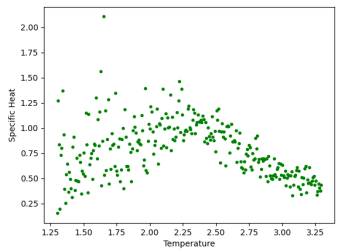
(a) lattice size 5X5 and sweep N= 100



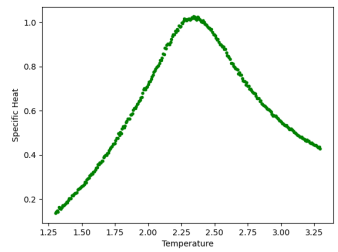
(b) lattice size 5X5 and sweep N= 10000



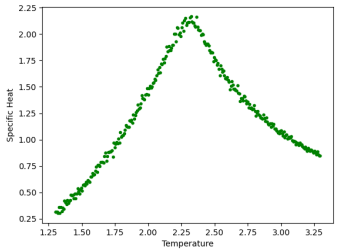
(c) lattice size 5X5 and sweep N= 100000



(d) lattice size 10X10 and sweep N= 100



(e) lattice size 10X10 and sweep N= 10000



(f) lattice size 20X20 and sweep N= 10000

Figure 2: Plots of specific heat as a function of Temperature for different lattice sizes and Monte Carlo sweeps

4 Conclusion

The simulation of 2D Ising model by using Metropolis Algorithm is an effective method in studying the ferromagnetic materials and estimate the critical temperature at phase transition. The drawback of this simulation is that it takes long time to run, especially for large size lattices. Therefore, the simulation needs more optimization methods.

Here are the references

[1] E. Ising, *Beitrag zur Theorie des Ferromagnetismus*, **31** (February, 1925) 253–258.

[2] L. Onsager, *Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition*, *Phys. Rev.* **65** (Feb, 1944) 117–149.

[3] W. Cai, *Handout 12. Ising Model* `http://micro.stanford.edu/~caiwei/me334/Chap12_Ising_Model_v04.pdf`, Feb, 2011. Accessed: 2023-05-11.

[4] *Ising model* `https://rajeshrinet.github.io/blog/2014/ising-model/`. Accessed: 2023-05-07.

[5] *Monte Carlo method applied on a 2D binary alloy using an Ising Model on Python* `https://towardsdatascience.com/monte-carlo-method-applied-on-a-2d-binary-alloy-using-an-ising-model-on-python-70afa03b172b`. Accessed: 2023-05-07.

[6] *scipy.optimize.curve fit* `https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.curve_fit.html`. Accessed: 2023-05-07.

[7] *Ising model in 2d wrong heat capacity* `https://stackoverflow.com/questions/49724370/ising-model-in-2d-wrong-heat-capacity`. Accessed: 2023-05-08.

[8] S. El-Showk, M. F. Paulos, D. Poland, S. Rychkov, D. Simmons-Duffin, and A. Vichi, *Solving the 3D Ising model with the conformal bootstrap*, *Phys. Rev. D* **86** (Jul, 2012) 025022.