Project 3: Numerical Statistical Mechanics

Elias Gutierrez[1, a)]
UCLA Physics and Astronomy, Knudsen Hall 475 Portola Plaza, Los Angeles, CA 90095

(Dated: 30 May 2017)

In order to simulate the 2D Ising model as accurately, I use the Metropolis-Hastings algorithm to generate the code with the absence of an external magnetic field with temperature points of 218; the size of the square lattice of 16; the amount of sweeps near the equilibrium point of 1000; and for the amount of sweeps of the Metropolis-Hastings algorithm of 1000.

I. INTRODUCTION

A. History

In 1946, the mathematician Stanislaw Ulam was playing solitaire by selecting a statistical example to approximate a combinatorial problem, and which he realized that the same idea could be used on computers to solve some physics problems.[1] Important contributions to the Monte Carlo simulations were developed over the next few years such as John Von Neumann and Ulam developing the Monte Carlo algorithms including sampling and rejection sampling; in the 1930's Enrico Fermi designed FERMIAC which is a Monte Carlo mechanical device which performs calculations; and in 1949 Nick Metropolis and Stan Ulam first published the basis of modern sequential Monte Carlo methods.[1]

B. Monte-Carlo Methods

In order to make the Monte-Carlo work is to generate "random" numbers where the algorithms would generate these "random" numbers that are deterministic but share the same random features on statistical tests.[2] There are two such generators that have these feautres which are the Linear Congruential Generator and the Lagged Fibonacci Generator.

The Linear Congruential Generator creates a sequence of numbers in the range of $[0, M]$ by using a recurrence:[2]

$$n_k = a \cdot n_{k-1} + b mod M, \tag{1}$$

where the seed n_0 is the first that determines the sequence.

The Lagged Fibonacci Generator uses the recurrence:[2]

$$n_k = a \cdot n_{k-\nu} + b \cdot n_{k-\mu} + c mod M, \tag{2}$$

where the seeds $n_0, n_1, ..., n_\mu$ determines the sequence.

C. Metropolis-Hastings Algorithm

Let $q(x, y)$ be the candidate-generating density where $\int q(x, y)dy = 1$ which means when the process is at point x, then the density generates a value of y from $q(x, y)$.[3] If $q(x, y)$ satisfies $\pi(x)q(x, y) = \pi(y)q(y, x)$ where π is the density, then the search is over.[3] If for the movement from y to x is not made enough where:

$$\pi(x)q(x, y) > \pi(y)q(y, x), \tag{3}$$

then there needs to be a probability of $\alpha(x, y)$ to be as large as possible with an upper limit of 1.[3] Therefore, plugging in this probability when $q(x, y)$ is satisfied which gives us $\alpha(x, y) = \pi(y)q(y, x)/\pi(x)q(x, y)$, then that means that:

$$\pi(x)q(x, y)\alpha(x, y) = \pi(y)q(y, x)\alpha(y, x) = \pi(y)q(y, x), \tag{4}$$

which makes $\alpha(x, y) = 1$.[3] The probability of move must be set to:[3]

$$\alpha(x, y) = min[\frac{\pi(y)q(y, x)}{\pi(x)q(x, y)}, 1], if \pi(x)q(x, y) > 0 \tag{5}$$

$$= 1, otherwise \tag{6}$$

This abstract concept is known as the Metropolis-Hastings algorithm, and summarizing how it works:[4]

1. Initiate the sequence of samples in a state σ_1 of your choosing, and successively generate states in the following way:

2. If σ is the current state, propose a new state σ' according a conditional probability distribution q, namely $q(\sigma'|\sigma)$ is the probability of proposing σ' given the current state is σ.

3. Accept the proposed state, namely add it as the next state in the simple sequence, with probability:

$$A(\sigma'|\sigma) = min(1, \frac{\pi_{\sigma'}}{\pi_\sigma}\frac{q(\sigma|\sigma')}{q(\sigma'|\sigma)}). \tag{7}$$

If the state is not accepted, in other words if it is rejected, add the current state σ to your sequence instead as the next state.

4. Repeat these steps for a large number of samples.

a) Electronic mail: blackcubes@ucla.edu.

D. Ising Model

The 2D Ising Model is a simple model of a ferromagnetic material with a phase transition.[4] The model consists of a 2D lattice $L \times L$ of spins $s_i \in \{-1, +1\}$.[4] Each spin interacts only with its nearest neighbors.[4] The energy is expressed as:

$$E(\{s_i\}) = -\sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i, \tag{8}$$

where $\{s_i\}$ is notation for the entire configuration of spins, H is the external magnetic field, and $\langle i,j \rangle$ implies a summation over all nearest-neighbor pairs.[4] We have normalized energy with J, spin with $\hbar/2$, and magnetic field with J/μ, where J is the exchange energy and μ is the atomic magnetic moment.[4] When the system is in contact with a heat bath at temperature T, the equilibrium probability density is the Boltzmann distribution:

$$\rho(\{s_i\}) = Z^{-1} exp(-E(\{s_i\})/T), \tag{9}$$

where the partition function Z is the sum of exponential factors $\exp(-E/T)$ over all possible configurations.[4] Below the critical temperature of $T_c = 2.2692$ is where the spins are preferentially aligned in a given direction; above T_c the spins have no mean orientation for $H = 0$.[4] To implement the Metropolis-Hastings algorithm for the 2D Ising model is by:[4]

1. Pick a random site i on the 2D lattice and compute the energy change ΔE due to the change of sign in s_i:

$$\Delta E = 2s_i(s_{top} + s_{bottom} + s_{left} + s_{right} + H), \tag{10}$$

where s_{top}, s_{bottom}, s_{left}, and s_{right} are the 4 nearest neighbors of s_i.

2. If $\Delta E \leq 0$ accept the move. If $\Delta E > 0$ accept the move with probability $A = exp(-\Delta E/T)$.

3. Flip the spin s_i if the move has been accepted.

4. Repeat steps 1-3 until you generate a large sample of spin configurations.

II. RESULTS

In the absence of an external magnetic field for the 2D Ising model on a square lattice of size $L \times L$ with periodic boundary conditions, and by utilizing the Metropolis-Hastings algorithm, the following results were obtained on python. When generating the following graphs, the amount of temperature points was 218 which is used to plot the various points for the given Ising model equations; for the square lattice, the size was a 16; the amount of sweeps near the equilibrium point was 1000 which shows where the graphs start to change; and for the amount of sweeps of the Metropolis-Hastings algorithm was 1000 which is before and after the equilibrium. These were the best values that I could obtain to generate the graphs especially for the two sweeps since the computation time was lengthy. Any more iterations of the sweeps such as 2000 would have gone on for a very long time without any results, and anything less than 1000 sweeps would have generated lousy graphs. The best I could achieve with decent computational time of 90 minutes was 1000 sweeps.

For the mean internal energy, it is defined by $U = \frac{1}{N}\langle E \rangle$ where $\langle E \rangle = \frac{1}{4}s_i(s_{top} + s_{bottom} + s_{left} + s_{right})$, and $N = L^2$ is the total number of sites.[4] The graph of the result is shown below:

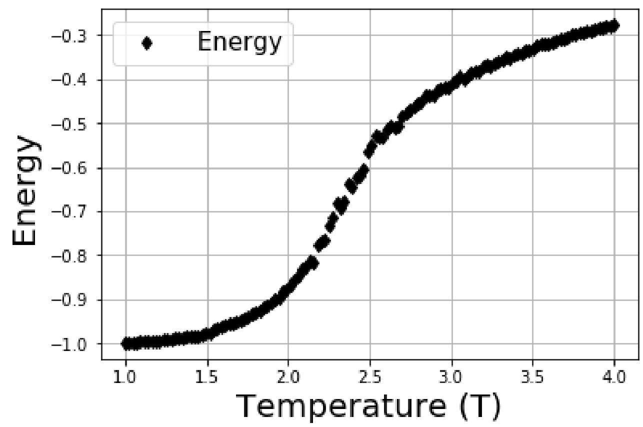

FIG. 1: Graph of the Mean Internal Energy versus Temperature

For the magnetization, it is defined by $M = \frac{1}{N}\langle S \rangle$ where $S = \sum_i s_i$ is the net magnetization.[4] For the Onsager's exact solution of the magnetization, it is defined by:

$$M(T) = [1 - sinh^{-4}(2/T)]^{1/8}, for T < T_c \tag{11}$$
$$0, for T \geq T_c. \tag{12}$$

Two graphs are presented showing the magnetization based on the 2D Ising model by itself, and comparison of the 2D Ising model estimate and Onsager's exact solution:

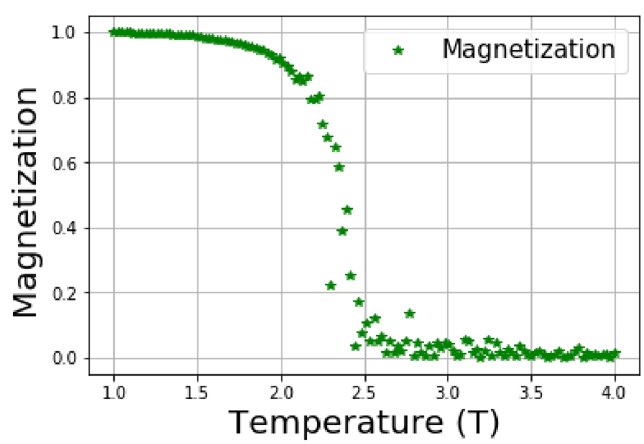

FIG. 2: Graph of the estimate Magnetization versus Temperature

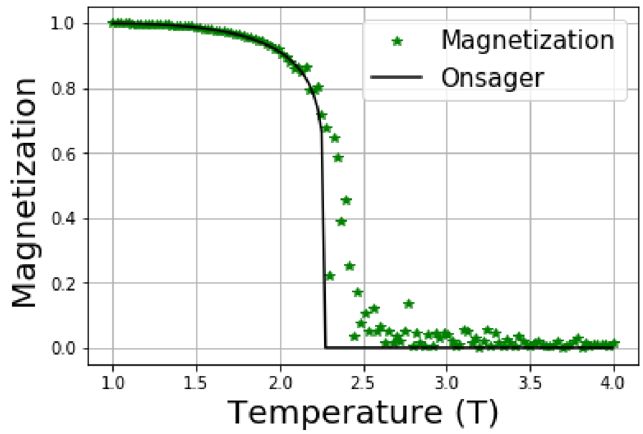

FIG. 3: Graph of the estimate Magnetization and Onsager's exact solution

The specific heat is defined by $C_H = \frac{1}{NT^2}(\langle E^2\rangle - \langle E\rangle^2)$.[4] The graph of it is presented below:

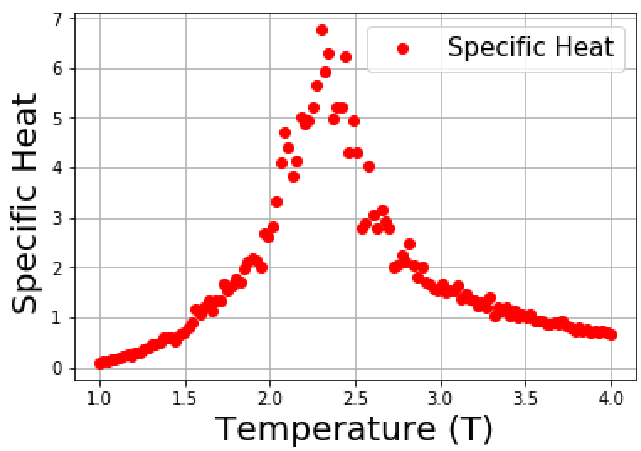

FIG. 4: Graph of the Specific Heat versus Temperature

The magnetic susceptibility (per lattice site) is defined by $\chi_T = \frac{1}{NT}(\langle S^2\rangle - \langle S\rangle^2)$.[4] The graph of it is presented below:

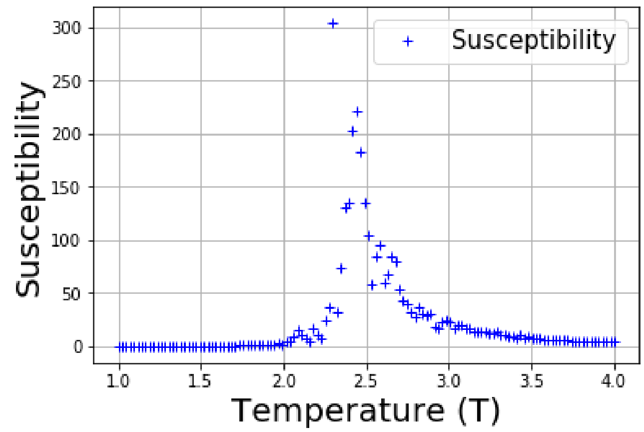

FIG. 5: Graph of the Magnetic Susceptibility versus Temperature

III. CONCLUSION

Using the Metropolis-Hastings algorithm shows that near the critical temperature T_c, the mean internal energy, magnetization, specific heat, and magnetic susceptibility undergo a phase transition. By utilizing the Metropolis-Hastings algorithm, it shows that it could be used as a close approximate value based on the comparison of Onsager's exact solution for magnetization. Yet, utilizing the algorithm to generate the simulations results in high memory intake which leads to lowering the values of the sweeps to calculate the results of the 2D Ising model.

IV. REFERENCES

[1]C. Andrieu, N. De Freitas, A. Doucet, and M. I. Jordan, Machine learning **50**, 5 (2003).
[2]P. J. Atzberger, .
[3]S. Chib and E. Greenberg, The american statistician **49**, 327 (1995).
[4]J. Samani, .