Project 4

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Abstract

In this report we have numerically approximated the 2D Ising model by using the Metropolis algorithm. We attempt to numerically calculate the critical temperature of a ferromagnet, and analyze the steps we took trying to reach this result. We started by studying a 2×2 lattice and later expanded to a $N \times N$ lattice after confirming that our first results, for the mean energy, mean absolute magnetization, heat capacity and magnetic susceptibility, corresponded with our analytical calculations. Conclution?

1 Introduction

In this project we will use the Monte Carlo method called the Metropolis algorithm in order to study the 2D Ising model, used to simulate ferromagnets as a funtion of temperature. By generating an arbritrary $N \times N$ matrix of spin-up and spin-down (± 1) values, we use the Metropolis algorythm to find the mean energy, the mean magnetization, the spesific heat and the susceptibility numerically.
To make sure the algorithm works properly, we started by studying a 2×2 lattice of spins in a system with temperature $T = 1$ and calculate both the analytical and numerical values. After confiming that they do we used them to study phase transitions at a critical temperature, for a few different system sizes, and to try to estimate an exact value for the temperature in which a transition would occure.

2 Theory?

2.1 The Ising Model

The model we will be using is the Ising model. It is a mathematical model of ferromagnetism, and is simplified in a 2D lattice S of binary spins s_i, j.

$$S = \begin{bmatrix} s_{0,0} & s_{0,1} & \cdots & s_{0,N} \\ s_{1,0} & s_{1,1} & \cdots & s_{1,N} \\ \vdots & \vdots & \ddots & \vdots \\ s_{N,0} & s_{N,1} & \cdots & s_{N,N} \end{bmatrix} \tag{1}$$

An example of a 4×4 lattice would be

$$\begin{array}{cccc} \uparrow & \uparrow & \downarrow & \uparrow \\ \downarrow & \uparrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \downarrow & \downarrow & \downarrow \end{array} \Leftrightarrow \begin{array}{cccc} +1 & +1 & -1 & +1 \\ -1 & +1 & +1 & -1 \\ -1 & +1 & +1 & +1 \\ +1 & -1 & -1 & -1 \end{array} \tag{2}$$

The total energy in the ising model is given by summing over the nearest neighbors, which represents the energy stored in an individual spin:

$$E = -J \sum_{<kl>}^{N} s_k s_l - \mathcal{B} \sum_{k}^{N} s_k, \tag{3}$$

with $s_k = \pm 1$, J is a constant expressing the strengt of the interaction between naboring spins and $\mathcal{B}$ is an external magnetic field. The $< kl >$ in the sum tells us that we only sum over the nearest neighbors, and N is the total number of spins.

The energy for a spesific configuration i is given by

$$E_i = -J \sum_{<kl>}^{N} s_k s_l. \tag{4}$$

The probability of finding the system in a given configuration i is given by the probability distribution

$$P_i(T) = \frac{e^{-\beta E_i}}{Z} \tag{5}$$

with $\beta = \frac{1}{kT}$, where k is the Boltzmann constant and T is the temperature. Z is the partition function for the canonical ensemble, given by a sum over all the microstates M,

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}. \tag{6}$$

The expectation value of the energy is given by

$$\langle E(T) \rangle = \sum_{i}^{M} E_i P_i(T) = \frac{1}{Z} \sum_{i}^{M} E_i e^{-\beta E_i}. \tag{7}$$

The mean magnetization is given by

$$\langle M(T) \rangle = \sum_{i}^{M} M_i P_i(T) = \frac{1}{Z} \sum_{i}^{M} M_i e^{-\beta E_i}. \tag{8}$$

The specific heat C_V is given by

$$C_V = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) = \frac{\sigma_E^2}{k_B T^2} \tag{9}$$

The susceptibility χ is given by

$$\chi = \frac{1}{k_B T} (\langle \mathcal{M}^2 \rangle - \langle |\mathcal{M}| \rangle^2) = \frac{\sigma_{\mathcal{M}}^2}{k_B T} \tag{10}$$

Table 1. List of configurations. Ising model, two dimentions

Number spins up	Degeneracy	Energy	Magnetization
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

In this paper we will be using periodic boundary conditions for all our calculations. This means that when looking at interactions between particles at the border of the matrixes, we assume that there exists theoretical particles above, below or to either side of the border particle, with the same spin as the particle on the opposite side.

2.2 Analytical solution of Ising model in two dimentions

A 2×2 Ising model on a square lattice with periodic boundary conditions have a total of $2^4 = 16$ states. The energy for all these different configurations are listed in the table below.

These values for the energy is used to calculate the partition function, 6, this calculation is quite simple and gives us

$$Z = 4(\cosh \beta 8J + 3). \tag{11}$$

Now that we have this we can find the expectation value 7,

$$\langle E \rangle = \frac{-32J \sinh \beta 8J}{Z} = \frac{-8J \sinh(\beta 8J)}{\cosh \beta 8J + 3}, \tag{12}$$

and the mean absolute value of the magnetic moment $|M|$8 (we will refer to this as the mean magnetization),

$$\langle |M|(T) \rangle = \frac{8(e^{\beta 8J} + 2)}{Z} = \frac{2(e^{\beta 8J} + 2)}{\cosh \beta 8J + 3}. \tag{13}$$

We also find the spesific heat C_V 9,

$$C_V = \frac{256J^2}{k_B T^2 Z}(\cosh \beta 8J - \frac{2\cosh \beta 16J - 2}{Z}) \tag{14}$$

and the susceptibility χ 10

$$\chi = \frac{32}{\beta Z}\left(e^{\beta 8J} + 1 - \frac{2}{Z}(e^{\beta 16J} + 2e^{\beta 8J} + 4)\right) \tag{15}$$

2.3 The Metropolis Algorithm

The Metropolise Algorithm is an algorithm for finding the most likely state of a system, by approximating the the probability of the system changeing in a specific direction as a probability for the transition and a probability for us accepting the transition.

$$W_{i\to j} = T_{i\to j}A_{i\to j} \tag{16}$$

In out case this means that we will mean that we need to find the probability of accepting a spin to be fliped. This is obtained by letting

$$A_{i\to j} = 1 \text{ if } \Delta E <= 0 \text{ or } e^{\beta\Delta E} \text{ if not.} \tag{17}$$

Where $\Delta E = E_j - E_i$. This means that we can set up a system, check it's energy, flip a random spin, and check it's energy again. If the energy has becom smaller like we want, the flip is accepted. If it is not, we randomly accept or decline it given by a uniform distribution, such that it is more likely to be accepted the less it increases the energy.

2.4 Phase transition

A phase transition is an abrupt macroscopic change when external parameters are changed. The point in which this change takes place is called the critical point, and many physical properties can be harder to describe around this point. An example of this is when the heat capasity C_v changes from rising along with an external rise in temperature to decreasing as the temperature gets higher. The same can happen with the susceptibility when the temperature rises. The temperature in which these properties changes, is the critical temperature T_c

2.5 Power law behavior

The heat capasity C_v, magnetization M and susceptibility χ can all be describes by different power laws around the critical temperature for an Ising model. In theories of critical phenomena [?] it is possible to find laws for all of these properties, as a function of the critical temperature and and the temperature of the system. For the mean magnetisation will be given by

$$\langle M(T)\rangle \sim (T - T_C)^{\beta} \tag{18}$$

where $\beta = \frac{1}{8}$. The heat capasity is given by

$$C_v(T) \sim |T_C - T|^{-\alpha} \tag{19}$$

where $\alpha = 0$, and the susceptibility is given by

$$\chi(T) \sim |T_C - T|^{-\gamma} \tag{20}$$

where $\gamma = \frac{7}{4}$. Lastly, it is possible to find that the critical temperature scales as a function of the lattice size N

$$T_C(N) - T_C(N = \infty) = aN^{-1/\nu} \tag{21}$$

Where a is a constant and ν is defined by the correlation

$$\xi(T) \sim |T_C - T|^{-\nu} \tag{22}$$

3 Method

First, we used the Metropolis algorithm, with the Ising model and periodic boundary conditions to calculate the mean energy, mean magnetization, heat capasity and susceptibility for a $2x2$ spin system, with temperature $T = 1$ and a $J = 1$. Then we computed the same values for a $40x40$, $60x60$, $80x80$ and a $100x100$ system, with temperature T ranging from $T = 2.0$ to $T = 2.3$. Finally we tried to use equation 21, with critical temperature obtained as the maximum point of the calculations earlier, to obtain an estimate of the critical temperature for our system.

4 Results

Quantity	Analytical	Numerical	Unit
$\langle E \rangle$	-1.99598	-1.99592	[J]
$\langle \lvert M \rvert \rangle$	0.99866	0.998665	[μ]
C_v	0.03208233	0.0325734	[J/K]
$\mathcal{X}$	0.00802013	0.00735754	*Dimentionless*

Table 2 Table of both analytical and numerical values. Note that all values are normalized by N^2, where the lattice is of size $N \times N$, and N in this case is 2.

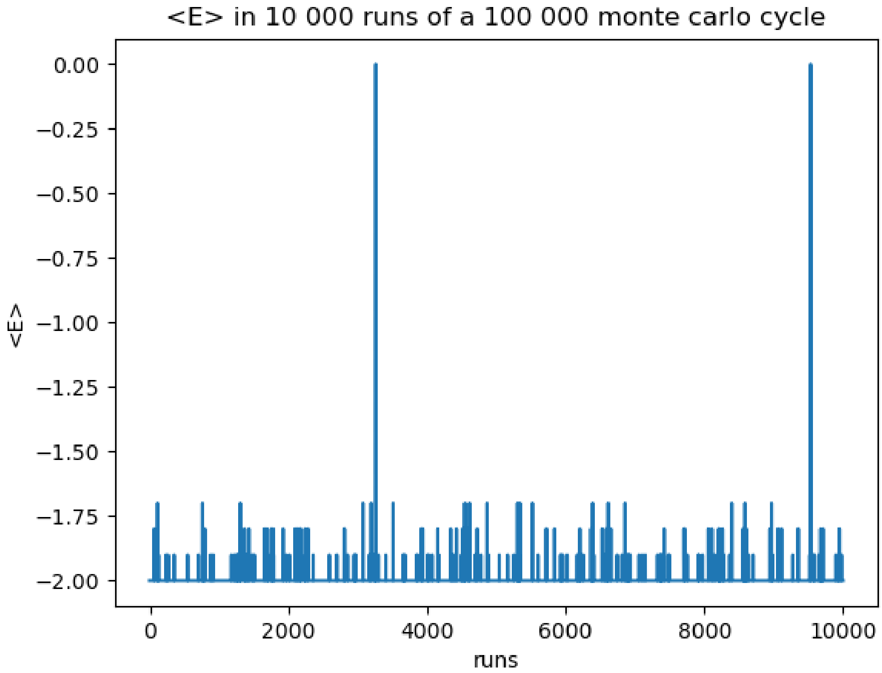

Figure 1 Graph over results from many runs of Monte Carlo, for the same number of cycles, to look at the consistancy of results. Also for a 2×2 lattice, same as in table 2 4

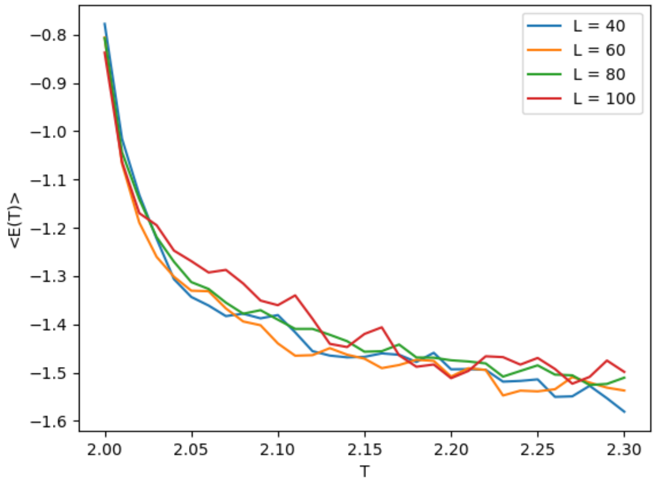

Figure 2 Plot of the mean energy of our system as a function of temperature for four different lattic sizes L.

The figures 2, 3, 4 and 5 show plots of the results obtained form analysing the Ising model over the temperature interval $T = [2.0, 2.3]$ with 30 points and 10000 Monte Carlo cycles for matrices with lattice size 40, 60, 80 and 100. We can clearly see that the mean energy in figure 2 decreases with the temperature, and is approximately propotional to $\frac{1}{T}$. The heat capasity shown in figure 3 looks like it, in general, is linearly decreasing with temperature. Figure 4 show the mean magnetization. Last, the susceptibility in figure 5 also lookes like it is propotional with T^{-1}.

5 Discussion

From our results while looking at the 2×2 lattice we can conclude that we get quite accurate results, except maybe for the susceptibility, but looking at the graph (1) we see that our calculations are not as consistant as we might want them to be, which might lead to irregular results later on.

When studying the phase transitions of our system, we would have expected the heat capasity and mean magnetisation to have a general trend up, and at some point switch and start decreasing. This is because of our expectation of there to exist a critical temperature where this switch would happen. However, the mean magnetisation we obtain is nothing less then chaos, and the heat capasity seems to have a general trend linearly down. Thus it makes it impossible to obtain a critical temperature for our later analysis of the critical temperature at the limit of the lattice going to infinity. What we would have done however, was to use equation 21, for all the different lattic sizes, an constructed a linear regression of the trend for the $T_C(L \to \infty)$. Then we could have used this to guess a value.

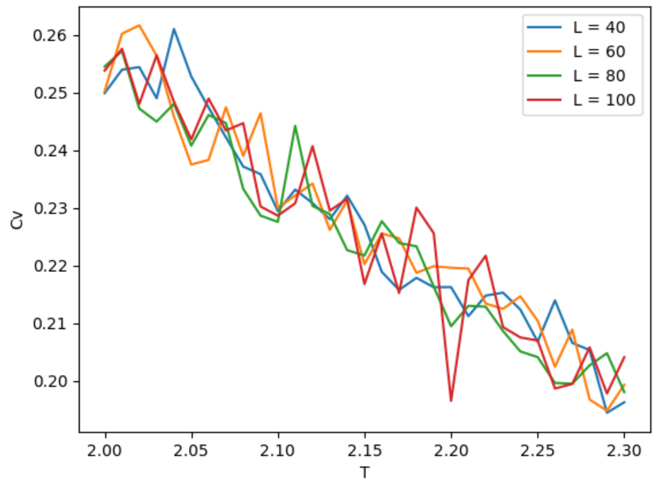

Figure 3 Plot of the heat capasity of our system as a function of temperature for four different lattice sizes L.

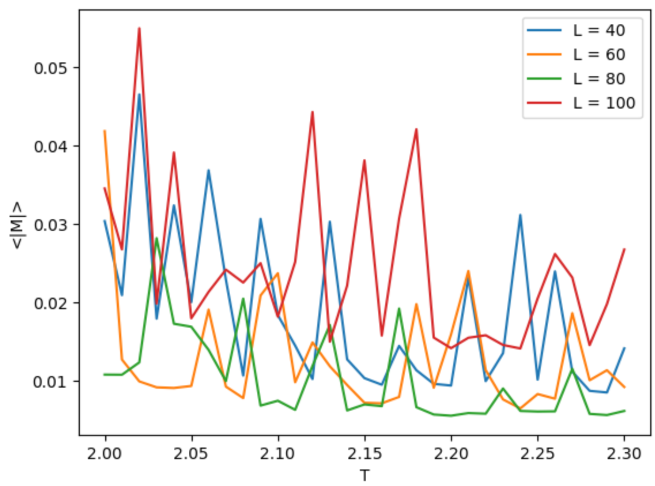

Figure 4 Plot of the mean magnetization of our system as a function of temperature for four different lattic sizes L.

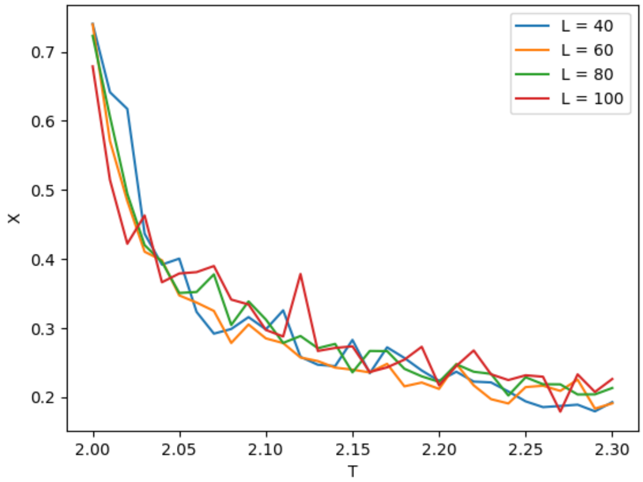

Figure 5 Plot of the susceptibility of our system as a function of temperature for four different lattic sizes L.

References

lectures https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Lectures/lectures2015.pdf