The Ising model and the Metropolis algorithm

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1 Abstract

The goal of this project is to compute the Curie temperature T_c as the system undergoes phase transition, with the help of the Ising Model and the Metropolis algorithm. Through the calculation of a specific lattice with the following parameters: energy E, absolute magnetization $|M|$, heat capacity C_V and susceptiblility χ, the analytical and numeric values where in good correspondence, given the right amount of Monte-Carlo cycles.

Contents

2 Introduction

In this project we will study a model that simulates phase transitions. The particular simulation we will study is known as the Ising model. This is a mathematical model in statistical mechanics used to simulate the magnetic properties of a material at a given temperature. The Ising model we are going to use is a simplified version where no external field interacting with the lattice.

We will be using the Ising model to simulate a two-dimensional ferromagnetic material. At a critical temperature , the Ising model will show a phase transition from a magnetic state to a non-magnetic state. This is then a binary system that holds only two values, in our case it will be spin up or spin down. Starting from this two dimensional lattice we will begin with describing the theory of the Ising model, and the workings of our algorithm of choice , the Metropolis-Hastings algorithm. Then we find the analytical expressions of partition function and the expectations values for E (energy), $|M|$ (magnetic moment), C_V(specific heat capacity) and χ (magnetic susceptibility) with respect to the temperature T, using periodic boundary conditions. These results will be used in the numerical computations to uncover the critical temperature, with the help of parallelization . At last the results will be discussed.

3 Theory

3.1 The Ising model

The Ising model consists of discrete variables that describe magnetic dipole moments in terms of spin up or spin down. In our simplified version, the Hamiltonian of a two dimensional model is given by the equation:

$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z, \tag{1}$$

where $\langle ij \rangle$ denotes a sum over the nearest neighbours of each spin. J is the coupling constant that describes the interaction between the neighbouring spins. We will assume J to be positive , in other words that we have a state of ferromagnetic ordering , which means the the neighbouring spins are aligned. This is because the energy will be lower The two dimensional Ising model on an infinite square lattice is analytically solved, by L. Onsager . The critical temperature was calculated to be

$$k_B T_C / J = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.2692. \tag{2}$$

3.2 Analytical expressions

First we start of by calculating the partition function, since it is needed to get analytical expressions for physical values like the susceptibility and heat

Table 1: The number of spins pointing up on a 2×2 lattice with corresponding degeneracies, energies and magnetizations. The energies are calculated with periodic boundary conditions.

spins	deg.	$E[J]$	M
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	$+8$	0
1	4	0	-2
0	1	-8	-4

capacity. For a 2×2 lattice with periodic boundary conditions, the possible energies and magnetizations are listed with the degeneracies in Table 1.

The energy is calculated from Eq.(1), and the magnetization is the sum of all the spins in the following equation,

$$M = \sum_{i=1}^{N} S_i^z, \tag{3}$$

where N is the total number of spins.

With the help of 1, we can calculate the mean energy $\langle E \rangle$, mean energy squared $\langle E^2 \rangle$,(absolute) magnetization $\langle |M| \rangle$ and $\langle M^2 \rangle$. The thermal average of a physical quantity is given by

$$\langle A \rangle = \frac{1}{Z} \sum_i A_i e^{-\beta E_i}, \tag{4}$$

where i is the number of micro states, $\beta = 1/k_B T$ and Z is the partition function, which in our case of 2×2 lattice is,

$$Z = \sum_i e^{-\beta E_i} = 4\left(3 + \cosh(8\beta J)\right). \tag{5}$$

We then get

$$\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-\beta E_i} = -\frac{1}{Z} 32 J \sinh(8\beta J), \tag{6}$$

$$\langle E^2 \rangle = \frac{1}{Z} \sum_i E_i^2 e^{-\beta E_i} = \frac{1}{Z} 256 J^2 \cosh(8\beta J), \tag{7}$$

$$\langle |M| \rangle = \frac{1}{Z} \sum_i |M_i| e^{-\beta E_i} = \frac{1}{Z} 8\left(2 + e^{8\beta J}\right), \tag{8}$$

$$\langle M^2 \rangle = \frac{1}{Z} \sum_i M_i^2 e^{-\beta E_i} = \frac{1}{Z} 32\left(1 + e^{8\beta J}\right). \tag{9}$$

From these expectation values, we can calculate the heat capacity at constant volume and the susceptibility of the system from the following relations (2):

$$C_V(T) = \frac{1}{k_B T^2}\left(\langle E(T)^2\rangle - \langle E(T)\rangle^2\right), \tag{10}$$

$$\chi(T) = \frac{1}{k_B T}\left(\langle M(T)^2\rangle - \langle M(T)\rangle^2\right). \tag{11}$$

3.3 Phase transitions

Phase transitions takes place in the critical point, which is marked by the critical temperature T_C. The material then goes from being a ordered ferromagnetic material to a disordered paramagnetic material.

The behaviour around the critical temperature can be connected to the thermodynamical potential of Helmholtz' free energy

$$F = \langle E\rangle - TS = -k_B T ln Z \tag{12}$$

where Z is the partition function , T is the temperature, k_B is the Boltzmann constant and S is the entropy. For simplification k_B will be set to one. This equation shows the struggle between energy minimization and the maximizing of entropy. For our two dimensional system, the desired outcome would be a minimzation of the energy. In this case, the minimal energy state is the ordered ferromagnetic state and also the the state of minimal chaos, hence minimal entropy.

The specific heat C_V is defined via the second derivative of F: $C_V = -\frac{1}{k_B T^2}\frac{\partial^2(\beta F)}{\partial \beta^2}$, where $\beta = \frac{1}{k_B T}$. Since the heat capacity and also the magnetic susceptibility χ diverges, the Ising model shows a second order phase transition. The same applies for the magnetic . Since both these magnitudes are temperature dependent , we also expect them to be affected when we reach T_C.

4 Algorithms

4.1 Monte-Carlo methods

Monte Carlo (MC) simulations has their basis on Markov chains, where the configuration evolves over time by multiplications of a stochastic matrix, and converges towards a steady-state.

MC simulations utilizes probability distribution , which in our case is Boltzmann statistics. In order to find all the probabilities, the partition function has to be calculated , which takes a lot of computer power , especially as the number of lattice points increase. This is where the Metropolis algorithm becomes useful, because the algorithm only takes in account the ratios between the probabilities , in this case the partition function cancels out and we only have to compute the Boltzmann factor.

4.2 The Metropolis algorithm

The Metropolis algorithm calculates the change in energy, ΔE, using this formula:

$$\Delta E = 2JS_l^1 \sum_{\langle k \rangle} S_k, \tag{13}$$

where S_l^1 is the value of the spin *before* it is flipped and S_k are the neighbour spins.

The Metropolis-Hastings algorithm can be broken down to the following steps.

1. The system is initialised by an initial state of energy E_0 and magnetization M_0 which can be generated randomly.

2. The initial system is changed by flipping the spin of a random site. One then calculates the energy of this new state E_{new}.

3. The difference in energy between the two states $\Delta E = E_{new} - E_0$ is calculated. Since we only take into account the closest neighbour interactions, there are only five possible values for ΔE when one spin is flipped. These are listed in the table above. This means, we can spare a lot of FLOPS by simply precalculating the factor $e^{-\beta \Delta E}$ for each temperature

4. If $\Delta E < 0$ the new configuration is accepted, meaning that the energy has lowered , and the system is moving towards an energy minimum. Note that the current value for energy and magnetization is updated. We therefore have to update the expectation values for E, E^2, M, M^2 and $|M|$, before the next MC cycle repeats.

5. If $\Delta E > 0$, compute and compare $w = e^{-\beta \Delta E}$ to a random number $r \in [0, 1]$. If $r < w$ the state is accepted, else the initial state is kept.

6. The expectation values are updated. And the steps 2-5 will be repeated until a satisfactory good steady state will be reached.

Other properties of the Metropolis algorithm is that it meets both ergodicity and detailed balance, which are requirements needed for convergence towards equilibrium.

As it takes some time for the configuration to converge towards equilibrium, the results should get better the more MC cycles that is used.

5 Code/implementation/ testing

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6 Results/Analysis

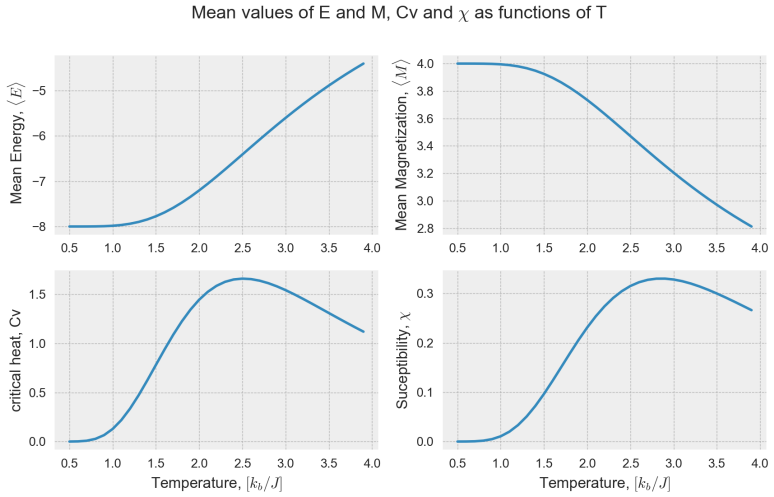

Figure 1: Plot that shows the numerical values Numerical (blue line) - RED-LINE the expectation value of the energy, absolute value of the magnetization, as well as the heat capacity and susceptibility for a 2×2 lattice as functions of temperature. This was calculated using 10^6 MC cycles without the system reaching equilibrium.

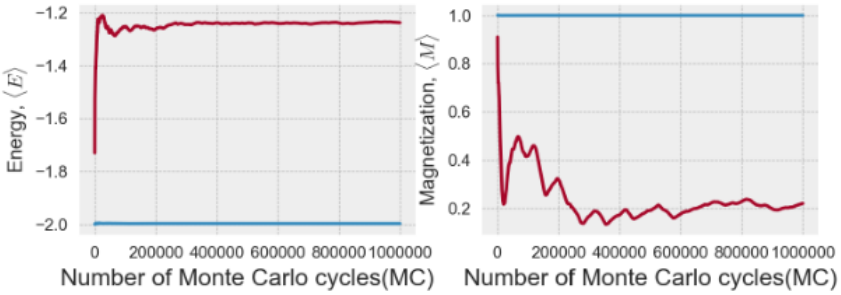

Figure 2: The expectation value of the absolute value of the energy and magnetization as a function of MC cycles for a 20×20 lattice. The simulation have been done for two different temperatures with and ordered initial condition . Ordered means that all spins starts pointing up ($S^z = 1$). Blue line represents $1J/k_B$ and red graph represents $2J/k_B$

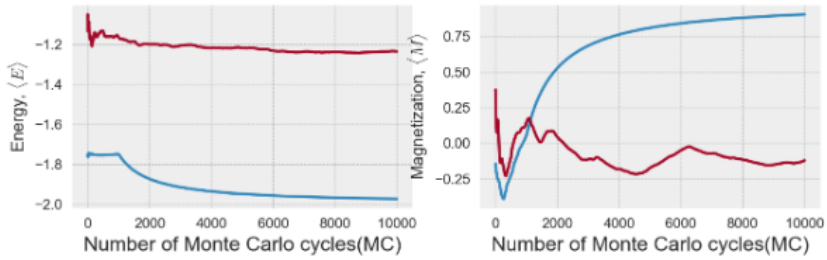

Figure 3: The expectation value of the absolute value of the energy and magnetization as a function of MC cycles for a 20×20 lattice. The simulation have been done for two different temperatures with initial disordered configuration. Disordered means that all spins starts configuration is chosen randomly. Blue line represents $1J/k_B$ and red graph represents $2J/k_B$

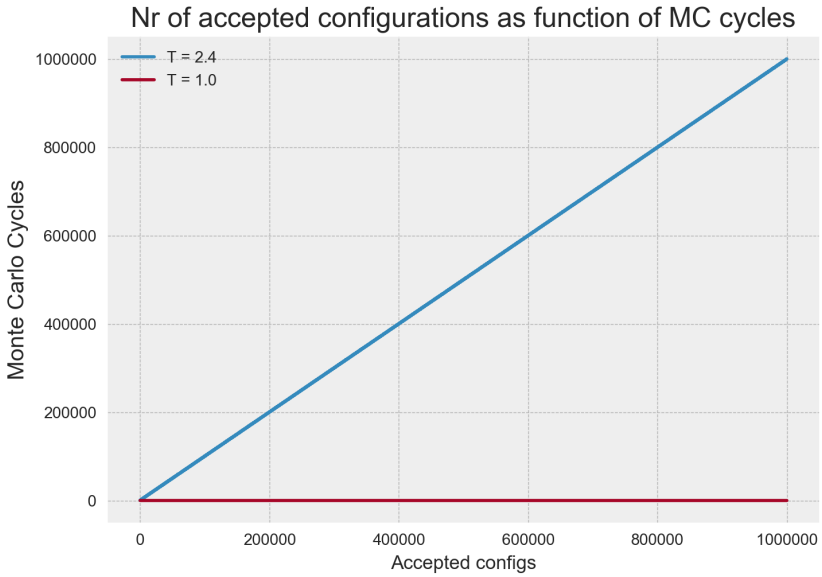

Figure 4: Figure showing that the number of accepted states for a high-temperature system ($T = 2.4$) has a proportional relation , while the accepted states for for a lower-temperature system ($T = 1$) has a constant relation at equilibrium.

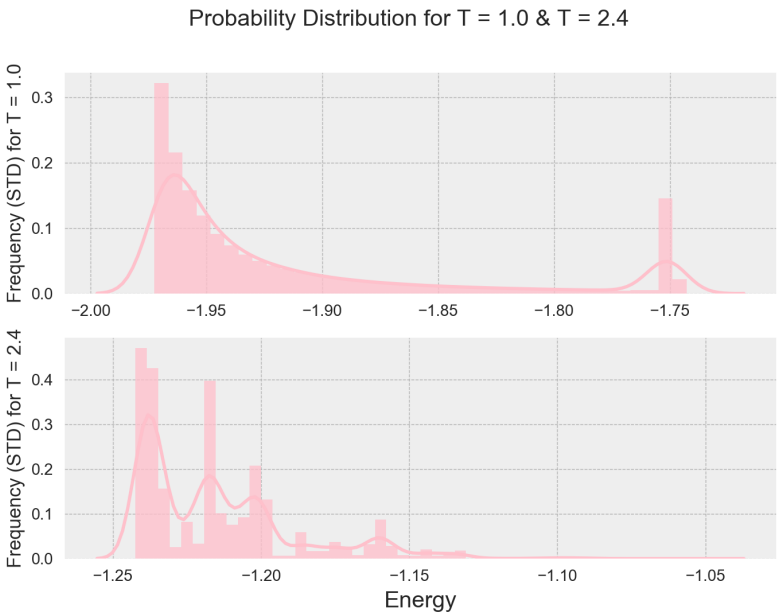

Figure 5: Probability densities for temperature $T = 1$ and temperature $T = 2.4$

6.1 Paralellization

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7 Discussion

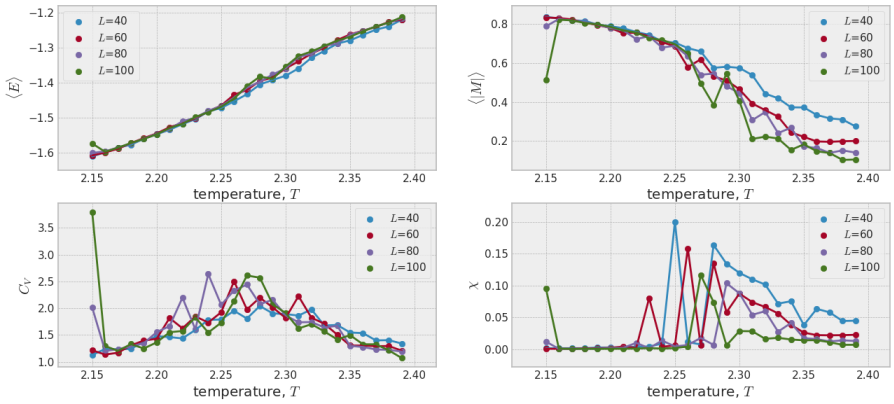

Figure 6: The mean energy, magnetisation, specific heat and susceptibility for larger spin lattices

through figure 2 3 we can see that the speed of reaching equilibrium depends on the initial value of low temperatures , but is less significant when it comes to higher temperatures. This is because for lower temperatures , the an ordered state is preferable. Order in this case means most the spins are pointing in one directions, also we have a ferromagnetic material. Starting from a lower temperature then means we have a an existing ordered system that is in other words in a equilibrium. Therefore for low temperatures equilibrium is reached instantaneously. Because of the accepting rule of the Metropolis algorithm, we stay in equilibrium. This is because the rule gives a small probability for flipping a spin when in steady-state, even if it did, it is highly likely it will be flipped back. From a disordered standpoint , or a higher temperature we are far away from equilibrium, since all configurations of spin will be accepted. This can be seen in the blue graphs of $T = 1.0J/k_B$. The configuration converges towards steady state, but will suddenly flip to a much more likely configuration and towards the more realistic equilibrium. The amount of MC cycles we required for equilibrium seems to be around $10^4 - 10^5$

COMMENT HERE (DIFFERENT VALUES FOR MC CYCLES)

The higher temperature of $T = 2.4J/k_B$,

COMMENTS ON CYCLES we see that the equilibration time is independent on whether the initial state is ordered or not. In this case we expect an almost non-magnetized configuration, that should be 50% of the spins pointing up, and the rest pointing down. We see though from Fig. **??** on page ?? that the magnetization is non-zero for the steady state. This follows from the small lattice size. For this lattice size, the critical temperature is still above $2.4J/k_B$. Thus, we do not expect an completely unordered state. The spins are still

somewhat correlated, and we are still in the ferromagnetic phase. This explains why neither the ordered nor the unordered configuration is the steady state, and both reach the steady state equally fast $\sim 10^5$ MC cycles. For temperatures above the critical temperature, we expect the unordered configuration to be closer to the steady state.

COMMENTS ON ACCEPTED STATES Figure 4 shows the number of accepted flips during 10^5 MC cycles plotted for temperature. As expected, few flips are accepted below the critical temperature in the ferromagnetic phase, on steady-state.That is why we see a constant line on $T = 1$ For higher temperatures, the amount of accepted states are high, higher than 50% due to the increase in disorder.

COMMENT ON THE CRITICAL TEMPERATURE

The top left picture of figure 6, shows that the energy increases with increasing temperature. This makes sense , because the structure gets more disordered.

This is expected, as the spin configuration becomes more disordered. We also see that the energy increases faster around the critical temperature for bigger lattices. The heat capacity seems to be bigger for large lattices around the critical temperature.

We think that Fig. **??** on page ?? show some reasonable results. This graph shows that the critical temperature gets closer to the analytical value as the lattice size increases. We also see that the phase transition become more visible, in the sense that one would expect the slope of the order parameter to approach infinity at the critical temperature. The paramagnetic to ferromagnetic phase transition in a 2D Ising model on a square lattice is continuous at the critical temperature, which is in correspondence with the theory. As for susceptibility, it peaks around the critical temperatures, as expected.

Due to the overwelming calculation time , only 10 000 cycles where used for this project. The results could have been better with more cycles

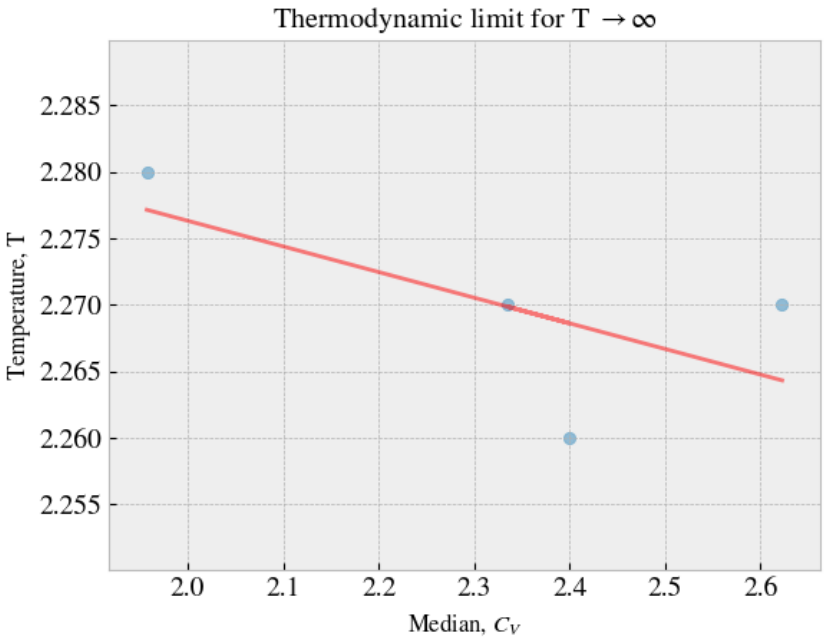

Figure 7: COMMENT METHOD HERE the critical temperature at $L \to \infty$ can be interpreted as the constant term, which is $T_C(L \to \infty) = 2.277 J/k_B$.

8 Conclusion

In this project we have studied the phase transition of a ferromagnetic material in a two dimensional square lattice. The Curie temperature was found using Monte Carlo simulations with the Metropolis algorithm. Using the calculated values of

$$T_C(L \to \infty) = 2.277 J/k_B, \tag{14}$$

By calculating the heat capacity for different lattice sizes, we could extract the critical temperature by locating the maximum of the heat capacity. EXPLAIN MORE ON YOUR METHOD

References

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[2] M. Hjorth-Jensen, Computational Physics Lecture Notes Fall 2019 (2019).

[3] L. Onsager, Phys. Rev. **65**, 117 (1944).