Two-dimensional Ising Model using Monte Carlo algorithm

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Abstract

This report aims to present how the Monte Carlo algorithm was used to carried out simulations of a two-dimensional Ising model on a $L \times L$ square lattice. The observables such as the magnetization, susceptibility, heat capacity and the energy are calculated for different lattice sizes. Phase transitions at the critical temperature are discussed for such magnitudes. Lastly a finite size scaling analysis is undertaken to determine the critical exponents. The results obtained from the simulation are compared to exact calculations to endorse the validity of this numerical process.

I. Theory

I. Background and Model

A ferromagnet is the material that have a preferred alignment of the atomic spins at certain conditions, and therefore an initial magnetic moment. The Ising model is used to investigate the properties of a two dimensional ferromagnet with respect to its magnetization and energy at varying temperatures.

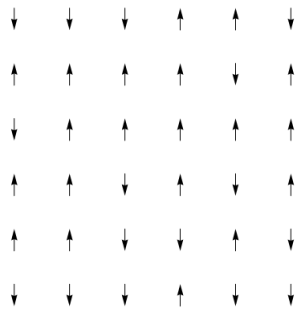

Figure 1: *2D lattice illustration of an Ising Model. The up and down arrows represent the positive and negative spins*

The Ising Model in two dimensions places dipole spins at regular lattice points while restricting their spin axis to be either up or down .(Figure 1). The lattice configuration is square with dimensions L and the total number of spins are $N = L \times L$. In its simplest form the interaction range amongst the dipoles is restricted to immediately adjacent sites (nearest neighbours). This produces a Hamiltonian for a specific spin site, i, of the form:

$$H_i = -J \sum_j s_i s_j \tag{1}$$

where the sum runs over the nearest neighbours of i. The coupling constant between nearest neighbours is represented by J while the s_i and s_j are the spin in consideration and the nearest neighbour spins. The nature of the interaction in the model is all contained in the sign of the interaction coupling constant J. If J is positive it would mean that the material has a ferromagnetic nature, which implies paralell alignment.J will take value +1 for the simulations and the values of the spins will be +1 for spin up and -1 spin down. Moreover J/K_b is taken to be 1, to analyze the observables in reduced units of the temperature. The relative positioning of nearest neighbours of spins is shown in Figure 2.

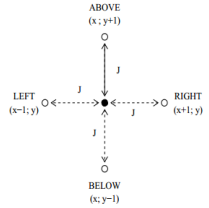

Figure 2: *Nearest neighbour coupling*

To maximize the interaction of the spins at

the edges of the lattice they are made to interact with the spins at the geometric opposite sites of the lattice. This is called periodic boundary conditions(pbc) and can be visualized better if we fold the 2D lattice into a 3D torus with spins being on the surface, as shown in Figure 3

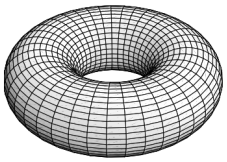

Figure 3: *3D torus representing the 2D lattice with pbc*

II. Computational issues

If the energy of each possible state of the system is specified (Equation 1), then the Boltzmann distribution (Equation 2) gives the probability for the system to be in each possible state, at a given temperature.

$$p(x) = \exp\left(-\frac{E(x)}{kT}\right) \tag{2}$$

Where k is the Boltzmann constant. Therefore macroscopic quantities can be calculated summing over the probabilities,namely,for any fixed state, x, the expected value of the energy and magnetization are given by:

$$\langle M \rangle = \frac{\sum_x M(x)p(x)}{\sum_x p(x)} \tag{3}$$

$$\langle E \rangle = \frac{\sum_x E(x)p(x)}{\sum_x p(x)} \tag{4}$$

where $M(x)$ is proportional to the "excess" number of spins pointing up or down:

$$M(x) \propto N_{\text{up}}(x) - N_{\text{down}}(x) \tag{5}$$

These calculation pose a drastic problem from a computational perspective. If we have two spin orientations and there are N spins, then we would have 2^N different states. As N becomes larger the computational treatment become intractable, if we use this manner. Thus, a better numerical alternative would be used to generate data over "representative states".

III. Monte Carlo method

An stochastic process make reference to the a random process that develop on time.Using Monte Carlo method we can make an stochastic interpretation of the sampling procedure to compute the observables of the Ising Model.The algorithm used is design around the principle of the Metropolis sampling.

III.1 Metropolis Algorithm

The algorithm implemented for this simulation is the Metropolis Algorithm [1].

Algorithm 1 General set-up of Metropolis Algorithm

```
Initialize the lattice (homogeneous or random distribution)
for iinN do
    Choose random spot on the lattice
    if ΔE < 0 then
        Flip spin at chosen position
    else

        if Random number < p(ΔE = 2E) then
            Flip spin at chosen position
        else
            Unchanged spin
        end if
    end if
end for
Add changes in the configuration of the lattice
if Monte Carlo loop is finished then
    Average of observables
    Output data
    End Program
else
    Continue the for loop
end if
```

This run will produce a set of observables for a given temperature. Since we are interested in find a phase transition with respect to the temperature is necessary to contain this procedure within a temperature loop in order to produce these observables in a range of temperature.

IV. Calculation of observables

The observables calculated were the Energy, Magnetization , and the fluctuations of them with respect to the temperature, which is reflected on the Heat Capacity and Susceptibility,respectively. They are computed as:

$$\langle M \rangle = \frac{\sum_x^N M(x)}{N} \tag{6}$$

$$\langle E \rangle = \frac{1}{2} \left\langle \sum_i^N H_i \right\rangle \tag{7}$$

$$C_v = \frac{\partial E}{\partial T} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{kT^2} \tag{8}$$

$$\chi = \frac{\partial M}{\partial T} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT} \tag{9}$$

$$\tag{10}$$

Therefore, through the main algorithm the observables that we should keep are:
$\langle E \rangle$, $\langle M \rangle$, $\langle E^2 \rangle$ and $\langle M^2 \rangle$

II. Observables's results

I. Simulation with one lattice size

The first simulation started from T = 0.5 to T = 10 in intervals of $\delta T = 0.1$, 100 Monte Carlo steps and a grid of 50×50, initialize with all the spins up.

•**Energy**:

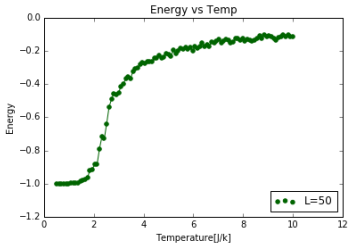

Figure 4: *Energy per spin for a lattice of 50×50 spins*

As can be seen in Figure 4 the energy stars at -1 where all the spins are up. Somewhere between $2 < T < 3$ there is sharp rise of the energy, showing that a transition to a non-ferromagnetic state has occurred, where the spins start to be oriented randomly as a result of the increasing of temperature.

•**Magnetization**

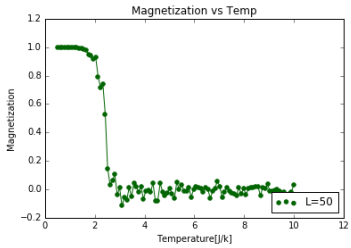

Figure 5: *Magnetization per spin for a lattice of 50×50 spins*

In Figure 5 is exhibited more clearly the transition temperature around 2.5 J/k reduced units. The magnetization starts at 1 an persisted for low temperatures in 1 because basically the Boltzmann (Equation 2) at low T tends to zero and then almost any spin would flip, as is shown in the Metropolis algorithm (Algorithm 1). Consequently this state initially magnetized will be maintain for low temperatures($T < 1$). After a critic temperature the magnetization suddenly drop to zero because the lack of the initial alignment.

•**Heat capacity and Susceptibility**

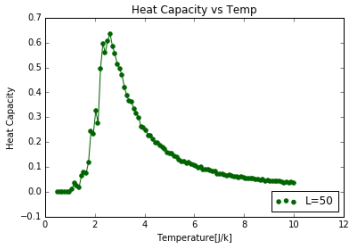

Figure 6: *Heat Capacity for a lattice of 50×50 spins*

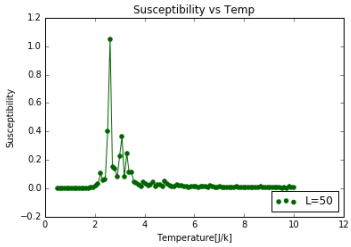

Figure 7: *Susceptibility for a lattice of 50×50 spins*

Figure 6 and Figure 7 shows the behaviour of the fluctuations of the magnetization and

the energy with the temperature. The peak, around a $2 < T < 3$ in both graphs reflects the abrupt change of such magnitudes near that T. It is seen a sharper peak in the susceptibility (**??**) resembling the more drastic change felt by the magnetization instead of the change in the energy.

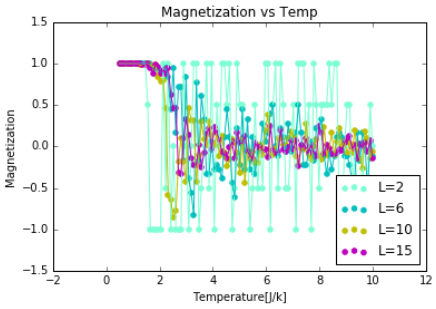

Figure 9: *Magnetization per spin for different lattice sizes (L)*

II. Simulation with 4 lattice sizes

The second simulation was carried out with different lattice sizes, ranging from 2 to 15, to visualize the effects of the boundaries and finiteness of the lattices.

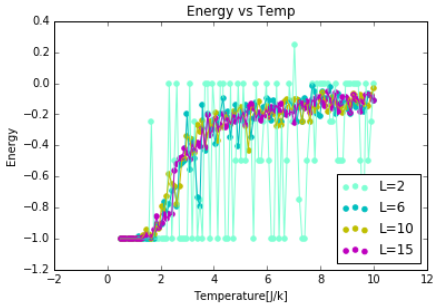

Figure 8: *Energy per spin for different lattice sizes (L)*

In this plot,it is depicted the effects of different lattice sizes in the energy of the system. Initially always the system have zero energy but then only the size of 10×10 and 15×15 show a similar and expected behaviour of Figure 4. Putting, on purpose, a lattice of $2x2$ we can show that such a system is constantly changing the phase in which it is, given by the fact of the very small amount of spins able to sustain a kind of order.

The same behaviour can be observed in the Magnetization plot Figure 9. The purple and yellow curve shows the better results, which is in concordance with their lattice's sizes. Even though those curves display fluctuations that are uncharacteristic for the model. This result in spontaneous flips of the spins, and this is an important effect that we have to deal in finite sizes, where there is a finite probability for this kind of behaviour to take place. This probability is clear that is inversely proportional to the lattice size. Corresponding fluctuations on the heat capacity and susceptibility, also can be observed in Figure 10 and Figure 11.

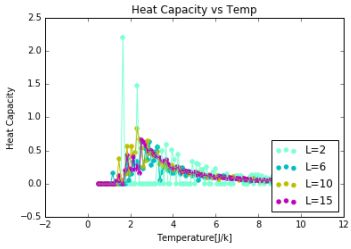

Figure 10: *Heat Capacity for different lattice sizes L*

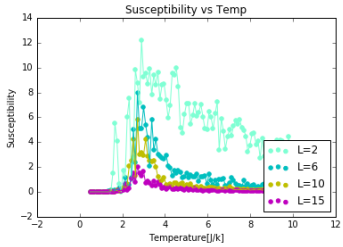

Figure 11: *Susceptibility for different lattice sizes L*

III. Exact Results

To evaluate the numerical process carried out, we need to compare with the exact solutions of the two dimensional Ising Model in the abscence of an external magnetic field ,proposed by Onsager in 1944 [2]. The Onsager solution gives the critical temperature,T_c, [3]:

$$\frac{kT_c}{J} = \frac{2}{ln\left(1+\sqrt{2}\right)} \approx 2.269 \tag{11}$$

In this results already shown the phase transition is somewhere around this temperature. The Onsager solution for the magnetization is given as [2]:

For $T < T_c$

$$M = \left[1 - \left[\sinh\left(ln\left(1+\sqrt{2}\right)\frac{T_c}{T}\right)\right]^{-4}\right]^{\frac{1}{8}} \tag{12}$$

And for $T > T_c, M = 0$. The comparison of my results with Onsager solution is presented in **??**:

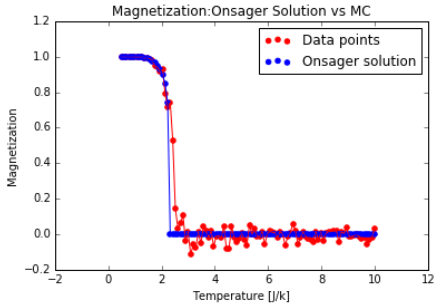

Figure 12: *Magnetization computed vs Exact solution*

IV. Critical behaviour

I. Finite size Scaling

One of the limitations that the Ising Model confronts us with is the finite size of the lattice. This results in a problem of recognizing the specific point at which the phase transition occurs. This effect is minimized by using periodic boundary conditions but would only be resolved if we where to consider an infinitely sized lattice as with the associated theoretical values for the phase transition(Onsager solution). It is thus necessary to use a construct that will allow us to extrapolate the respective theoretical value given the limited resource of a finite sized lattice. For that purpose,the procedure of finite size scaling (fsc) method [4] is used. Lets define a critical exponent which will give us information about the nature of the divergence near the critical temperature. The critical exponent λ, is given by $\lambda = \lim_{t->0} \frac{ln|F(t)|}{ln|t|}$. This can be rewritten as $F(t) \sim |t|^{\lambda}$ where $t = T - T_c$. This exponent is also important because it offers a more universal characteristic for differing data collected.

The critical exponents relevant to the Ising Model are as follows:

$$\begin{aligned} \text{Correlation length} &: \xi(T) \sim |T - T_c|^{-\nu} \\ \text{Magnetization} &: M(T) \sim |T - T_c|^{\beta} \\ \text{Heat Capacity} &: C_v(T) \sim |T - T_c|^{-\alpha} \\ \text{Suseptibility} &: \chi(T) \sim |T - T_c|^{\gamma} \end{aligned}$$

Since the correlation length when the finite system is approaching the critical temperature can be understood as the size of the system itself then the critical exponent ν can be also applicable to the lattice size L. Therefore $L \sim |T_c(L = \infty) - T_c(L)|^{-\nu}$, and then we can express the above exponents in terms of the lattice size.

$$\xi(T) \sim |T - T_c|^{-\nu} \to L \tag{13}$$

$$M(T) \sim |T - T_c|^{\beta} \to L^{-\frac{\beta}{\nu}} \tag{14}$$

$$C_v(T) \sim |T - T_c|^{-\alpha} \to L^{\frac{\alpha}{\nu}} \tag{15}$$

$$\chi(T) \sim |T - T_c|^{\gamma} \to L^{\frac{\chi}{\nu}} \tag{16}$$

The results attempting to compute such critical exponents was using the four lattices sizes presented in the previous section, namely ,$L = 2, L = 6, L = 10, L = 15$. This calculation was done by taking the peak values of data collected of observables and plotting a ln-ln grapgh that should yield a straight line with the slope equal to the respective critical exponents, since ν=1 for a two-dimensional lattice.

•**Results**:

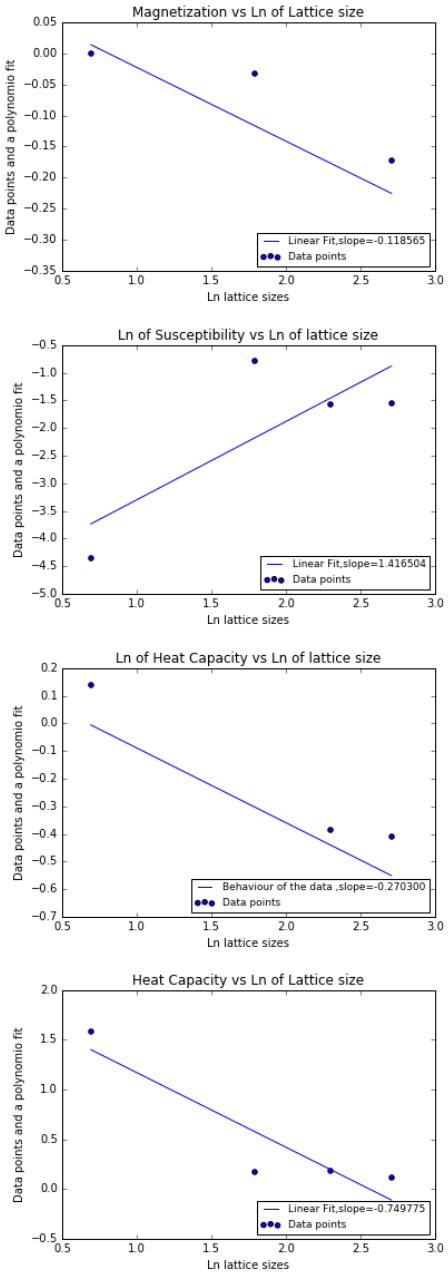

Figure 13: *Plots obtained for the calculation of the critical exponents*

The third graph for the Heat Capacity, isn't a straight line and shows a curvature. The reason is that α is zero in the 2D Ising Model and should rather be interpreted as $C_v \sim C_o \ln(L)$[5], as is better shown in the last one, where one of the points lie on the line. This results are summarized in the following table:

Table 1: *Calculated and theoretical critical exponents*

Quantity	Exponent	fsc	Theoretical
Magnetization	β	0.1185 ± 0.0071	0.125
Susceptibility	γ	1.4165 ± 0.3092	1.75
Heat Capacity	C_o	0.7497 ± 0.1026	0.500

II. Hoshen-Kopelman algorithm

In this section, is going to be described the cluster algorithm applied to speed up the Ising model computation, mostly when the slow down effect is taking place, near the critical temperature.The Hoshen-Kopelman Algorithm [6]is a simple algorithm for labeling clusters on a grid, where a grid is a regular network of cells, where each cell may be either "occupied"(spins up)or "unoccupied"(spins down). The HK algorithm is an efficient means of identifying clusters of contiguous spins. The general idea of the H-K algorithm is that we scan through the grid looking for spins up, for example. To each spin position we wish to assign a label corresponding to the cluster to which the spin belongs. If the spin has zero aligned neighbors, then we assign to it a cluster label we have not yet used (it's a new cluster). If the spin has one aligned neighbor, then we assign to the current cell the same label that have that neighbor (they're part of the same cluster). If the cell has more than one aligned neighboring cell, then we choose the lowest-numbered cluster label of such neighbors to use as the label for the current cell. A short description of it is:

Algorithm 2 Short description of Hoshen-Kopelman algorithm

```
for i in number of rows do
    for j in number of columns do
        Set the top and left neighbours of the current cell
        if left neither top are aligned with the current cell then
            Create a new label for that position
            if left is aligned but top not then
                Accept left neighbour to the cluster with probability 1-p
                if top is aligned but left not then
                    Accept top neighbour to the cluster with probability 1-p
                    if left and top neighbours are aligned with the current cell then
                        Choose the minimun label between them
                    end if
                end if
            end if
        end if
    end for
end for
```

The magnetization after applying this algorithm looks like:

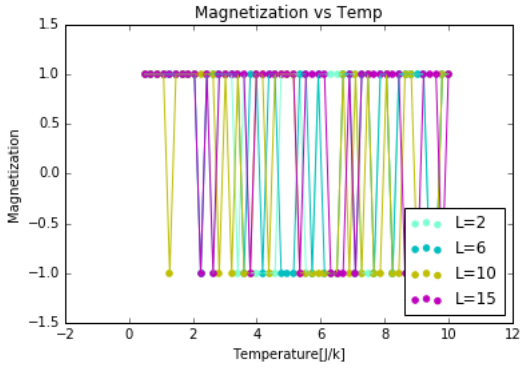

Figure 14: *Magnetization vs temperature*

V. Conclusions

In this report was exhibited Monte Carlo simulations for 2D Ising model. To do this the Metropolis algorithm was implemented. The dependence of the energy, magnetization, specific heat, and magnetic susceptibility of the system on temperature and different lattice sizes were calculated for 2D Ising model. The results were in agreement with the exact solutions for this case investigated by Lars Onsanger. Therefore the numerical results produced by the Monte Carlo simulation compare favourably with the theoretical results and are a viable and efficient alternative to an exact calculation. The requirements for producing accurate results are to consider large lattice sizes and a large number of Monte Carlo steps. A finite size scaling analysis was undertaken to determine the critical exponents for the observables. These where in acceptable range with respect to the theoretical exponents, considering the small lattice sizes,used for this. Finally, the Hoshen-Kopelman Algorithm was implemented to speed up the slow down effect that affect the simulation time when the temperatures are near the critical temperature.

Acknowledgements

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References

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