Ising Model

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Abstract. In this paper we study the behaviour of the well known "Ising Model" on a 2D lattice in its exact form and in the approximation of mean field theory. We look for phase transition and dynamical points of interest in the system, considering different parameters. The system is evolved trough Metropolis and Wolff algorithms, and we compared the numerical simulation with the analytical solution given by the exact Hamiltonian and the approximated one given by the mean field theory.

Keywords: Ising Model · Complex Systems · Phase Transition · Mean Field Approximation · Metropolis Algorithm · Wolff Algorithm

1 Theoretical introduction and predictions

1.1 Ising model

The Ising model is based on a D-dimensional discrete lattice. We will analyze the $D = 2$ case. The lattice can be pictured with a matrix, every entry is identified with two coordinates $[i, j]$ and the value of a site can be 1 or -1 [1]. The nearest neighbors of the site $[i, j]$ are formally: $[i + 1, j]$, $[i - 1, j]$, $[i, j + 1]$, $[i, j - 1]$. We define the *Hamiltonian*, a function representing the energy of the system, depending on the configuration:

$$H = B \cdot \sum_{i=1}^{N} S_i - J \cdot \sum_{<ij>} S_i \cdot S_j \tag{1}$$

where B is an external field, and J the coupling constant representing the interaction between the sites. Note that the interaction is considered only between the nearest neighbors[2].
We can define different thermodynamic variables, one of the most important is the average magnetization:

$$m = \frac{1}{N} \cdot \sum_{i=1}^{N} S_i \tag{2}$$

where N is the total number of sites of the lattice. The magnetization is important since it can identify a so called *phase transition*, i.e. a change in the

[1] We will call the entries as "spin" for known historical reasons.
[2] Short-range interaction.

behaviour of the system, that occur for a specific value of the temperature parameter T, called *critical temperature* T_c. Above this temperature the symmetry of the system is preserved and the magnetization is close to zero. Below T_c the system should go trough a spontaneous symmetry breaking, creating clusters of single-valued spin and increasing the module of the total magnetization.

1.2 The mean field theory

A useful approach to the Ising model seen above is the mean field theory. Consider the mean field Hamiltonian:

$$H_{mf} = B \cdot \sum_{i=1}^{N} S_i - J \cdot \sum_{<ij>} S_i < S_j > \tag{3}$$

where the symbol <> is the average of the quantity inside the bracket. This is the Hamiltonian of a system where the spin $[i, j]$ does not *see* his nearest neighbors as they are, but as a mean of the magnetization on the entire system. Since $< S_j >= m$ we can write:

$$H_{mf} = B \cdot \sum_{i}^{N} S_i - \frac{J \cdot m \cdot \gamma \cdot \sum_i S_i}{2} \tag{4}$$

where γ is the number of nearest neighbors (that in our case is 4). Working on the equation we can write the Hamiltonian in the form:

$$H_{mf} = h_{eff} \cdot \sum_{i=1}^{N} S_i \tag{5}$$

where

$$h_{eff} = B - 2 \cdot J \cdot m \tag{6}$$

In this way the analytic solution for m is much more easy (the partition function is easily factorizable), and we can make predictions under the approximation of mean field theory. One of them, is a phase transition individuated by the order parameter m at the critical temperature of $T_c = \frac{4 \cdot J}{K_B}$. In two dimension the mean field approach is a useful tool to predict the behaviour of the system (it can predict qualitatively the phase transition), but the value of T_c obtained does not correspond to the one found by the exact Ising model solution.

1.3 Micro and macro phase space

Microscopic phase space We can define a *microscopic* phase space of the system which consists in the ensemble of all the possible spins configurations. If we have a system of dimension $N \cdot M$, the phase space will have $2^{N \cdot M}$ elements. Considering a system that evolve with the *metropolis algorithm* (1.4), we look for **fixed points**, points that do not move in the phase space under any evolution. If

we consider the probability defined in equation 9, we can already conclude that there will always be a possibility for the spin to change his value i.e. there are not fixed points for the system, independently from the parameters (mainly from T). We could face the task to find basin of attraction and investigate stability for different temperatures, but as suggested by thermodynamics, we prefer to introduce a different phase space, discussed here below. The main reason to do this, is the high dimensionality of the system that makes really difficult a visualization and a deeper study.

Macroscopic phase space In order to avoid the difficulties that arise from a high dimensional phase space, we introduce a new one based on macroscopic variables. The most efficient observable for our aim is the magnetization. Different points in the microscopic phase space correspond to the same value of magnetization and this help us to simplify the analysis of the system. Following a similar reasoning used before, we can assert that theoretically there are no fixed points in the macroscopic phase space, since there is always a non-null probability to change the macroscopic variable, the magnetization. Nevertheless, we can look for basins of attraction. From the theoretical studies done on the 2D Ising model by Onsager and on the mean field approach, we know the relation between magnetization and temperature when the system is at the equilibrium. Equilibrium is a condition that we can reach only numerically trough Monte Carlo methods, since we do not have the equations for the dynamic of the system. At equilibrium we compute the quantity of interest in order to confront them with the theoretical predictions. Therefore, we want the theoretical curves (for example the one in the $M - T$ plane) to be basins of attraction for the evolution of our system.

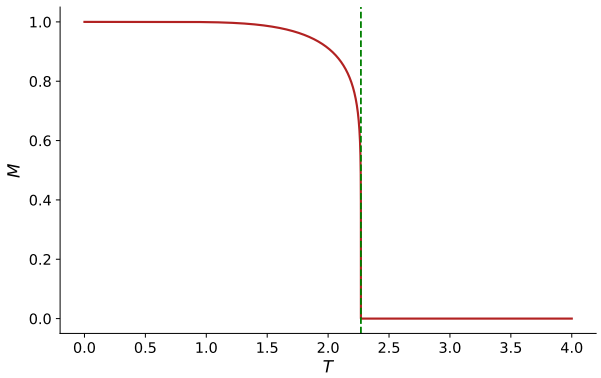


Fig. 1: Relation between magnetization and temperature at equilibrium founded by Onsager. Here is reported only the positive semi-plane for M.

For the 2-D Ising model, with $B = 0$, the theoretical relation between M and T at the equilibrium is (see Fig. 1):

$$m = \begin{cases} \pm[1 - sinh^{-4}(2\beta J)]^{\frac{1}{8}} & \text{if } T < T_c \\ 0 & \text{if } T \geq T_c \end{cases} \tag{7}$$

Below T_c, for each temperature, we have two values of magnetization that should be actractors. Above T_c the two points *merge* and become one. This is what we call a **phase transition**. The equation 7 has been found by Onsager in 1944, together with the value of the critical temperature: $T_c = \frac{2}{log(1+\sqrt{2})}$.
For the 2-D Ising model with $B = 0$ approached with the mean field, the theoretical relation between M and T at the equilibrium is:

$$m = tanh(\gamma J \beta m) \tag{8}$$

This relation does not give us a function ready to plot, indeed the equation can be solved graphically (see Fig. 2).

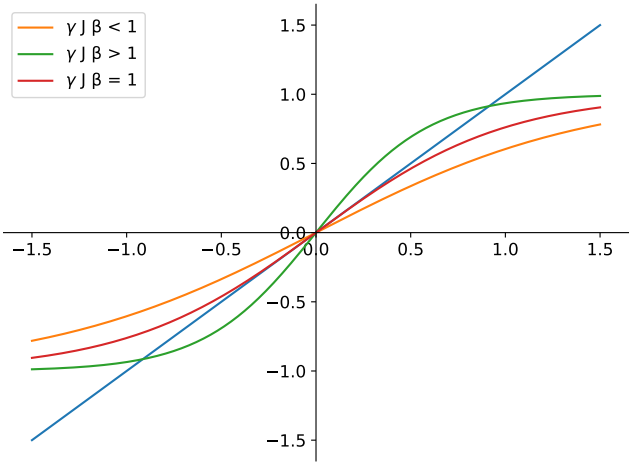


Fig. 2: Graphical resolution of equation 8

We can individuate three cases:

- $\gamma J\beta > 1$: there are three solutions. Two of them are symmetrics, the other is zero. The zero solution is not a physical solution since it does not minimize the energy[3].
- $\gamma J\beta = 1$: is the transition point and the solution is zero.
- $\gamma J\beta < 1$: there is only one solution in zero.

[3] It is an unstable solution.

In this case, the qualitative behaviour of the system is the same (presence of a phase transition), but the numerical value for T_c is different [4].

1.4 Computational methods

We describe here the methods used to evolve the system.

Metropolis algorithm After arbitrarily initializing the system, consider its configuration as a_0. Randomly, a point in the lattice is chosen and the spin is flipped. The idea of the method is to identify a probability function $f(\mathbf{X}_i)$ dependent on the state of the system, and accept the new change with a probability:

$$p = min(1, \frac{f(\mathbf{X}_{i+1})}{f(\mathbf{X}_i)}) \tag{9}$$

For reasons deriving from statistical mechanics, we choose as probability function an object called *Boltzmann factor*:

$$f(\mathbf{X}_i) = e^{-\beta H_i} \tag{10}$$

where $\beta = \frac{1}{K_b T}$, K_b is a constant and T is a parameter of the system that represents its temperature. Thus, the Metropolis algorithm promotes changes that reduce the energy of the system, but allows changes that increase energy with a certain probability.

Wolff algorithm This algorithm is based on cluster flipping. First the system is arbitrarily initialized and then a cluster is identified from a random site and eventually flipped. To do this the algorithm remember the direction of the chosen spin and put it onto a list. Then it looks at all the neighbors and add to the list the ones that has the same direction of the old spin with a probability

$$p = 1 - e^{-2\beta J} \tag{11}$$

and flip them. The process is iterated until there are no spin left in the list. In the algorithm 1 the pseudo-code is shown.

[4] Note that the mean-field is still an approximation.

Algorithm 1: Wolff Algorithm

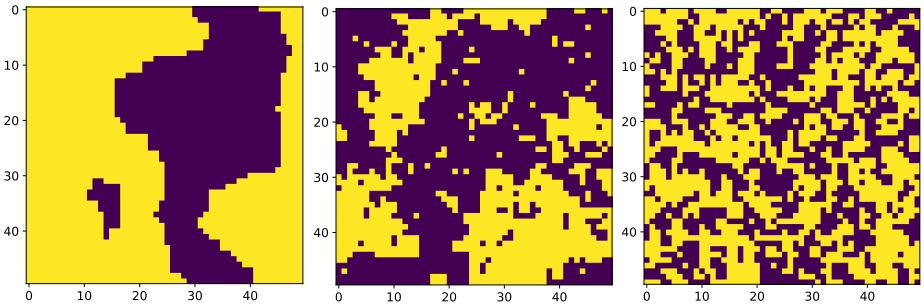
```
pick a random spin;
remember its direction as oldSpin;
push it onto a list "toFlip" of spins to flip;
while there are spins left in toFlip do
    remove the first spin;
    if it has not been flipped in between then
        flip it;
        for each of its neighbors do
            if the neighbor is in the oldSpin direction then
                with probability p, put it on the stack;
            end
        end
    end
end
```

2 Numerical simulation

For all the situations we present we set $J = 1$, $B = 0$ and $K_b = 1$. Moreover we used periodic boundary conditions.

2.1 Ising phase transition

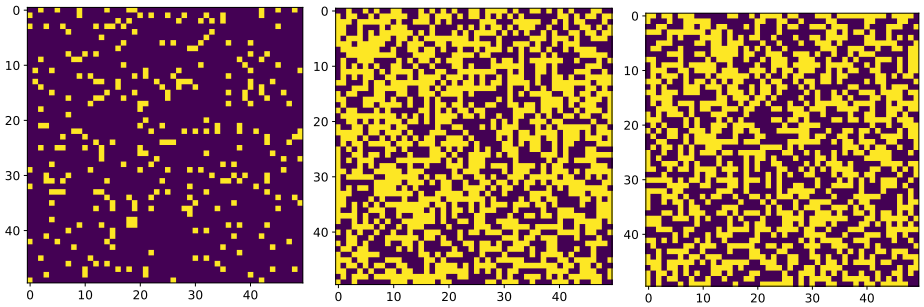
We choose the magnetization as order parameter to identify a phase transition. After a adequate number of "steps" of the computational method used, the system reach an equilibrium, hence also the magnetization. The evolution and the final state will depend from the parameter of the model: the temperature. We report the state of the system, after a certain number of steps, corresponding at three different values of the parameter that represent adequately the possible situations.



(a) $T < T_c$ (b) $T = T_c$ (c) $T > T_c$

Fig. 3: Final configuration at different temperatures obtained with **metropolis** algorithm.

We can observe (Fig. 3) that at low temperature the system create big clusters, and their size increase as the temperature decrease. At high temperature the system is stuck in an disordered state and it is not able to maximize the absolute value of the magnetization. At $T = T_c$ the behaviour is not well defined. We repeat the same process, but this time using the mean field approach.



(a) $T < T_c$ (b) $T = T_c$ (c) $T > T_c$

Fig. 4: Final configuration at different temperatures obtained with **metropolis** algorithm in mean field approximation.

Below the critical temperature the system is able to reach a fully magnetized state, but in this case the clustering process does not take place since the spins are "blind" at their neighbors.
Furthermore, we plot the absolute value of magnetization at the equilibrium state as a function of the temperature (Fig. 5) to individuate the two phases of the system. This time, we used the Wolff algorithm for computational time reasons.

We can see that, around the theoretical value of T_c predicted from the analytic

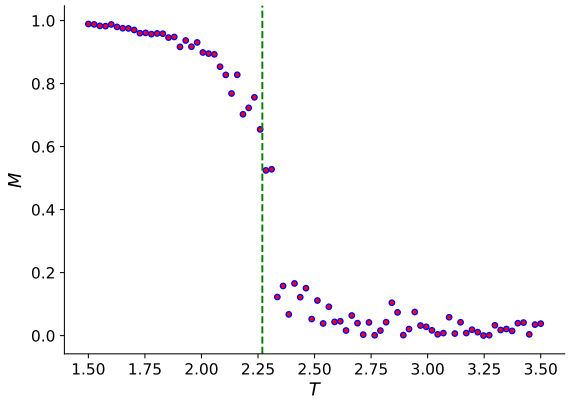


Fig. 5: Relation between magnetization and temperature at equilibrium obtained by simulation with **Wolff algorithm** for the exact Hamiltonian. The green dashed line represent the theoretical value of the critical temperature.

solution, the magnetization fast decreases and, after a certain temperature, it stabilizes around the zero.
In order to verify that the theoretical curve is a basin of attraction, we plot the state of the magnetization in function of the temperature for each step (Fig. 6).

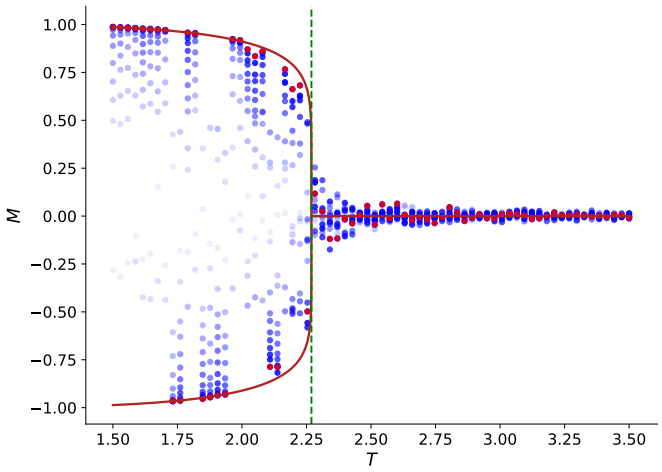


Fig. 6: Evolution of the magnetization to the equilibrium using the exact Hamiltonian, the red lines represent the analytical solutions. For the simulation the **Wolff algorithm** has been used.

In Fig. 6, the evolution of the magnetization can be visualized thanks to the density of the points that increase with the progress of the steps. In the plot it is clear that for each temperature the magnetization is attracted by the theoretically predicted value. We can then conclude that the evolution merge to this basin.

We repeated the simulation using the mean field approach. In Fig. 7 is shown the theoretical curve of the magnetization, found by sampling the transcendental equation (Eq. 8), and the evolution of the magnetization has been performed with the metropolis algorithm for different values of the temperature parameter.

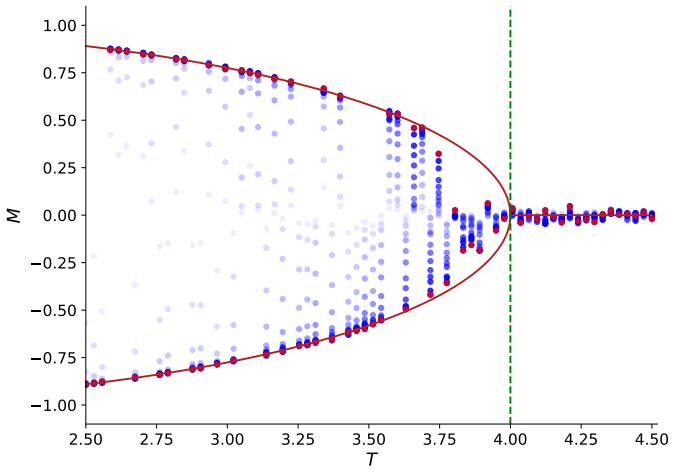


Fig. 7: Evolution of the magnetization to the equilibrium using the mean field approximation, the red lines represent the analytical solutions. To evolve the system **Metropolis algorithm** has been used.

We can see that for temperatures far away from T_c the evolution of the magnetization approaches to the theoretical curve. Close to T_c this convergence is harder.

3 Conclusions

We performed the evolution of a NxM dimensional binary system. We applied two different algorithms, the Metropolis one and the Wolff one. Both are based on simple rules of acceptance or rejection of a change and use a particular function, the Hamiltonian, which represents the energy of the system and depends on the temperature. Both the algorithms present a probabilistic step in their structure. Studying the system from a macroscopic point of view, we investigated the behaviour of the magnetization. We saw that, depending on the temperature parameter, the system presents different behaviours, individuating a phase transition that has a precise physical meaning. Below a critical temperature the system breaks the symmetry of the problem, and orients most of his spins in a verse, creating a state that is called magnetized. Above the critical temperature the system conserve the symmetry and stays in a disordered state, maintaining close to zero the value of the magnetization. We also analyzed the mean field model approach, that is an approximation of the Ising model. We confirmed its analytical solution, that predicts a similar qualitative behaviour. We indeed found a transition between two phases, a magnetized one and a non magnetized

one. For the MF model we found a different T_c from the one of the exact Ising model, and not well located. Indeed in Fig. 7, we can see that the transition from magnetized and non magnetized condition is smoother and our results do not overlap properly with the analytical solution of MF near the T_c. This can be due to the fact that close to this temperature the system could need more time to find the equilibrium. In a further work, the MF simulation could be performed in a smaller sub-domain of T, centered on T_c, and with more repetitions of the algorithm.

References

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