A Monte Carlo Implementation of the Ising Model in Python

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Abstract

This article explores an implementation of the 2D Ising model using the Metropolis algorithm in the Python programming language.

The goal of this work was to explore the scope of behaviours this model can demonstrate through a simplistic implementation on a relatively low-end machine.

The Ising model itself is particularly interesting as it demonstrates relatively complex behaviours of ferromagnetics e.g. the second-order phase transition in spite of its simplicity.

To study the specifics of this model several parameters were measured (namely the net magnetization and energy, the specific heat and correlation function) and a visualization of the grid was implemented.

The simulations demonstrated an easily observable phase transition near critical temperature on a 100×100 Ising grid with the measured parameters behaving nearly as predicted by the exact solution developed for this model.

1 Theory

1.1 Introduction

Ferromagnetics are a class of materials that can retain magnetization in absence of an external magnetic field. Such materials exhibit long-range ordering on an atomic level resulting in formation of domains - areas where unpaired electrons have identical spins. Each such domain has a relatively strong magnetic field. In unmagnetized materials domains with opposite alignments cancel each other's fields out, but through exposure to an external magnetic field nonzero net magnetization can be achieved.

At high temperatures thermal motion competes with the tendency for dipoles to align. When the temperature is raised to a point called the Curie temperature, the system can no longer sustain spontaneous magnetization and a second-order phase transition occurs.

The simplest model that describes ferromagnetism and this phase transition is the two dimensional Ising model.

1.2 Model

The model itself is a square lattice, each cell containing a value of either "1" or "-1", representing an electron's spin. Each spin interacts only with its nearest neighbours. To eliminate the effects of lattice boundaries, it is folded into torus [3] (the spins at opposite geometric edges are considered neighbours). In absence of an external magnetic field interaction between two dipoles "i" and "j" is given by the following formula:

$$E_{ij} = -J\sigma_i\sigma_j \tag{1}$$

Where J is the coupling constant, σ_i and σ_j are values of spins at sites i and j. Therefore the total energy E_k of a spin k is found as:

$$E_k = -J\sigma_k \sum_i \sigma_i \tag{2}$$

Where σ_i is a neighbouring spin.
The partition function Z is given by [1]:

$$Z = \sum_i e^{\frac{-E_i}{kT}} \tag{3}$$

Where k is the Boltzmann constant, T is the temperature, E_i is the total energy of the system in the respective microstate.

The two-dimensional model with no external field was analytically solved by Lars Onsager, showing that the model undergoes a phase transition at the critical temperature given by [5]:

$$T_c = \frac{2J}{k \ln(\sqrt{2} + 1)} \tag{4}$$

The spontaneous magnetization that occurs at temperatures lower than T_c was shown to be [1]:

$$M = [1 - \sinh^{-4} \frac{2J}{kT}]^{\frac{1}{8}} \tag{5}$$

Where k is the Boltzmann constant and J is the coupling constant.

1.3   Simulation

The Ising model is rather hard to evaluate numerically as the number of possible states for an NxN grid is 2^N. It is for this reason that the model is often simulated using the Monte Carlo method.

The most often used Monte Carlo algorithm used for this model (and by far the simplest one) is the Metropolis-Hastings algorithm, where each step a spin is chosen at random (so as to satisfy ergodicity) and flipped (its value changed to the opposite) under these conditions [4]:

1. If flipping the chosen spin k leads to a decrease in its energy E_k given by formula 2, then it is flipped.

2. If flipping the chosen spin k does not lead to a decrease in its energy, then it is flipped with the probability of $e^{-\frac{\Delta E_k}{kT}}$ where ΔE_k is the change in energy arising from flipping the spin.

1.4   Calculated Values

To evaluate the model's behaviour quantitatively the following values were measured:

- M - the average magnetization of all the spins on the grid.

- E - the average energy of all the spins of the grid.

- c_v - the specific heat of the grid, given by [6]:

$$c_v = \frac{1}{T^2}[\langle E^2 \rangle - \langle E \rangle^2] \tag{6}$$

- $G(r)$ - the correlation function between two spins σ_i and σ_j, r units apart from one another given by [6]:

$$G(r) = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle^2 \tag{7}$$

2   Implementation

The model was implemented in Python. An $n \times n$ numpy array was used as the Ising grid. To simplify calculations, both the magnetic coupling constant J and the Boltzmann constant k were taken to be 1, so the "true" temperature can be found as:

$$T_K = \frac{TJ}{k} \tag{8}$$

The Metropolis algorithm was implemented according to the outline given in section 1.3. while satisfying the periodic boundary conditions. Through trial-and-error it was found that, for a 100×100 grid, 150 steps of 10000 Metropolis loops were enough to achieve a stable state, yielding acceptable results in reasonable time.

In addition to calculating the values listed in section 1.4 , two visualizations using Matplotlib [2] were implemented as well - one allowing to see the end state of the grid and another showing the average values of spins on the grid throughout the simulation.

Three following methods were used for the simulation:

1. Start from a randomized grid for every value of temperature and record the final state.

2. Start from a randomized grid and reduce the temperature every 150 steps, recording the end state at every temperature, without resetting the grid.

3. Start from a ground state (where every spin is the same) and raise the temperature every 150 steps, recording the end state at every temperature, without resetting the grid.

3   Results

The implemented model successfully demonstrates a visible phase transition at around the calculated critical temperature using any of the methods listed in section 2.
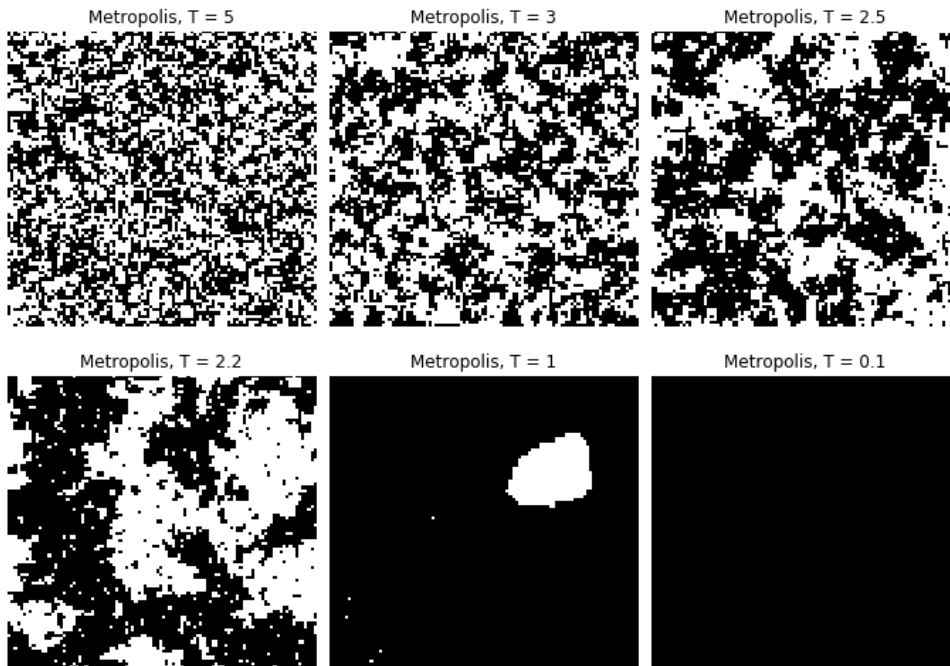

Figure 1: Final configurations of grids achieved through method one.

Figures 1 and 2 demonstrate the phase transition achieved through the first method. Figure 2 clearly shows the process of the grid falling into a ground state from a configuration of several large clusters. The states where the grid is composed of these large clusters are relatively stable and require quite a lot of iterations to fall into a ground state, the 150 steps given in all experiments sometimes proving insufficient. The third method listed in section 2 avoids these metastable states as there is no way for such clusters to form at a low temperature in a grid composed of identical spins.
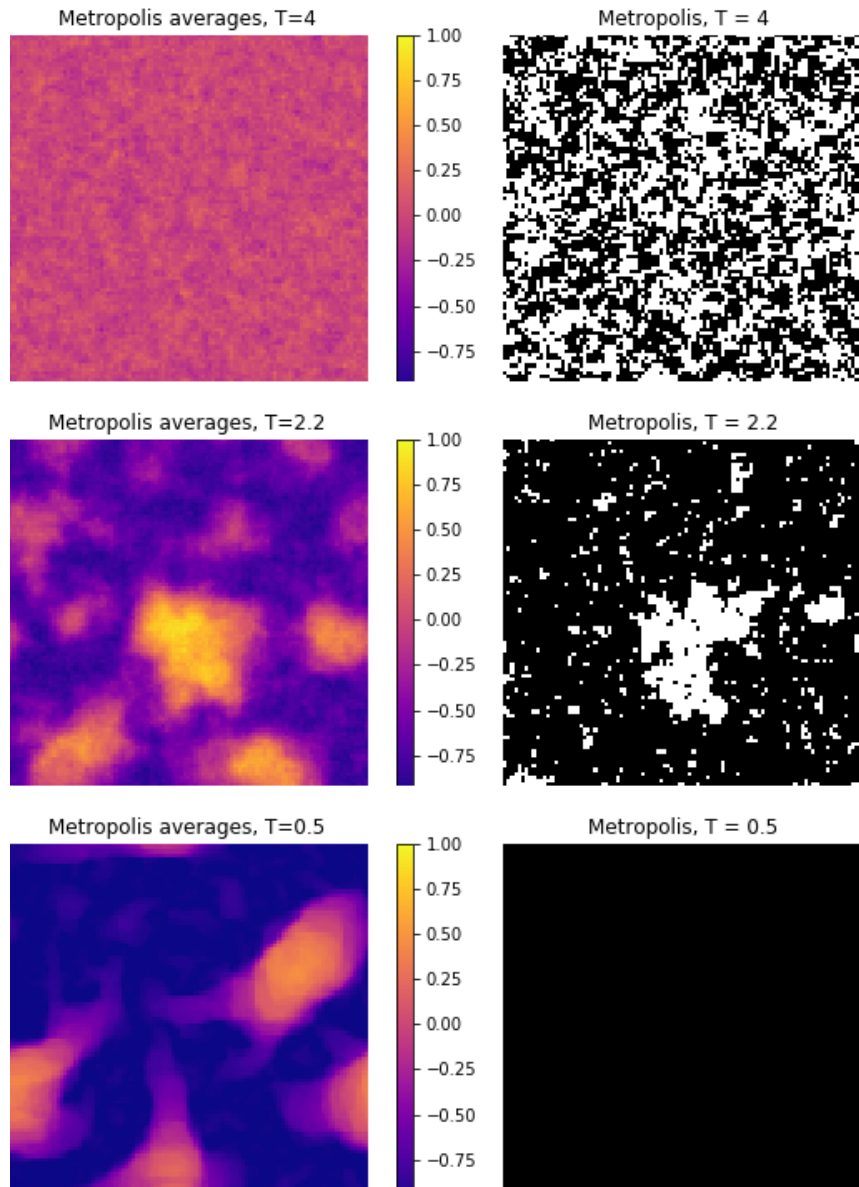

Figure 2: Final configurations and heatmaps of spin averages of grids achieved through method one. Note the progression of clusters vanishing in the bottom left image.

The results for energy of spins (presented in figure 3 below) clearly shows the predicted phase transition between two distinct phases with the low-temperature state having the lowest energy and the high-temperature state having the highest. All the methods outlined in section 2 produced nearly identical results, the only difference being the energy of the low-temperature state. This value is consistently lower in experiments produced by the third method as there are no metastable states that increase the mean energy through interaction between boundary spins.
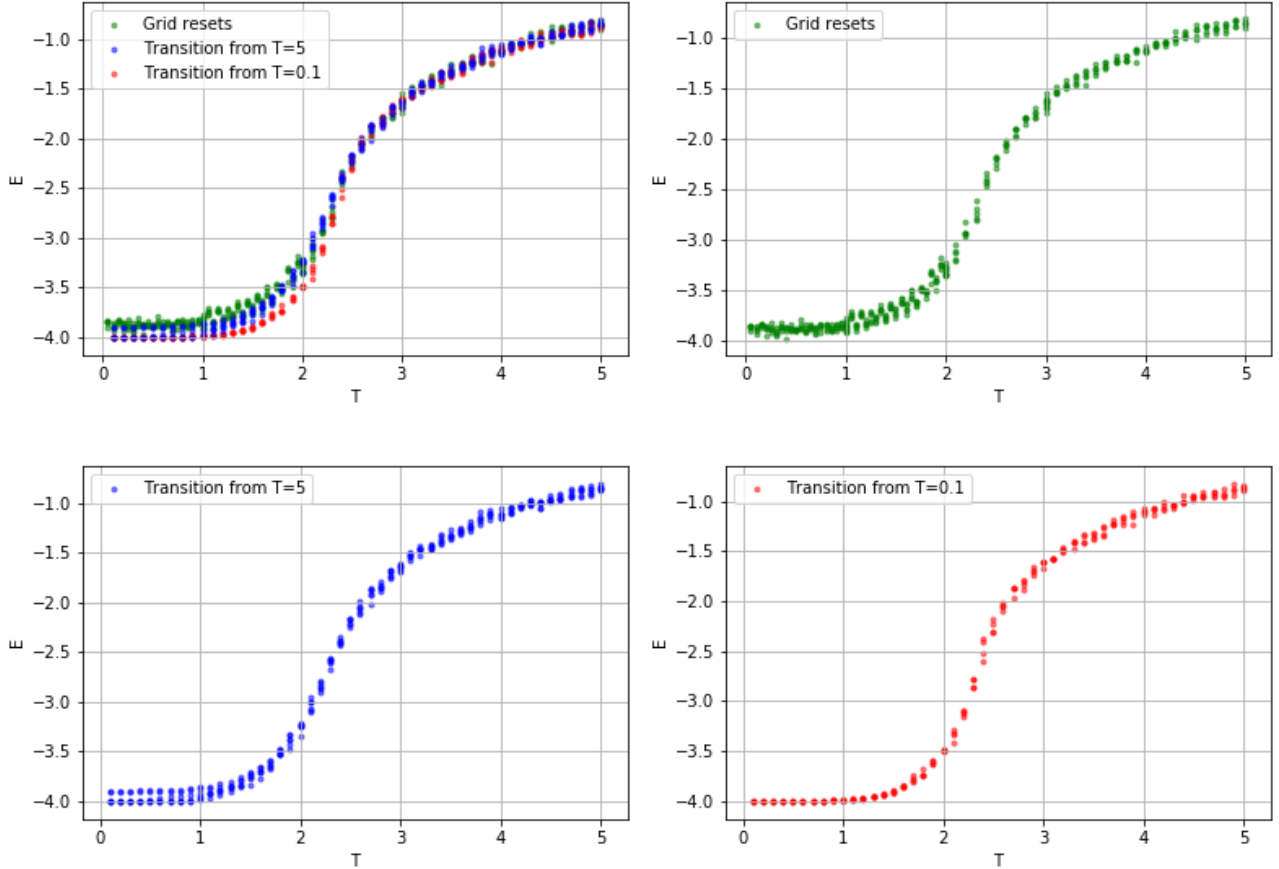
Figure 3: Plots of the average energy of spins as a function of temperature. Note the inflection point at around the critical temperature.

Results for the magnetization value differed significantly between methods (see figure 5 below). The first two methods produced results drastically deviating from the analytical solution, but nevertheless demonstrated the spontaneous symmetry breaking of the phase transition. This deviation is also caused by the presence of metastable states in configurations obtained through methods 1 and 2. Such states can possess any average magnetization between −1 and 1 as shown by the second and third plots in figure 5. The reason for this issue, as stated in the second paragraph of this section, is insufficient time for the system to fall into a truly stable state. Once again, the third method experiences no such problem, almost perfectly matching the analytical prediction.
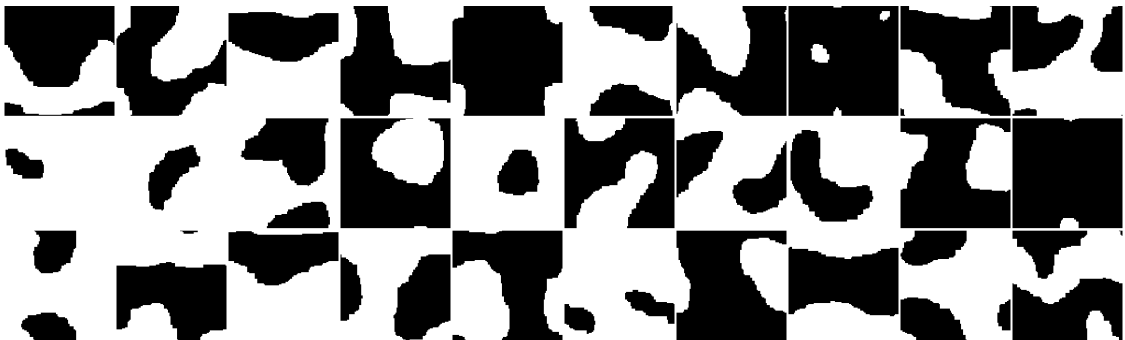

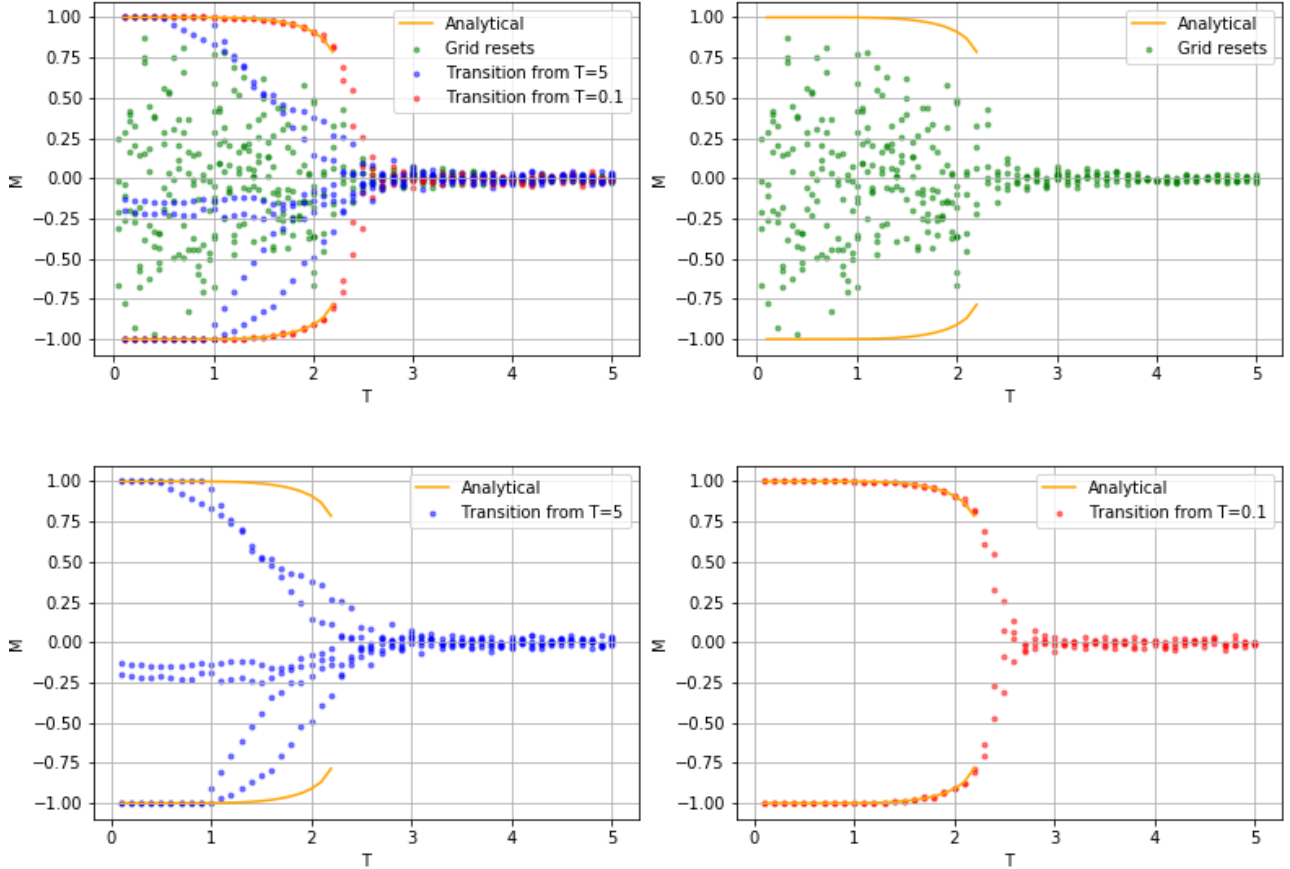Figure 4: Several configurations showing the possible shapes of the metastable states.

Figure 5: Plots of the average magnetization of spins as a function of temperature. The orange lines denote the value obtained through equation 5.

For calculating the specific heat only the second two methods were used. Both produced similar results with a peak located at critical temperature (see figure 6). The second method had an artifact where the specific heat peaked at zero temperature. Once again, the presence of metastable states is the cause, as the difference $\langle E^2 \rangle - \langle E \rangle^2$ is quite large due to a considerable number of spins with differing values, which causes, in tandem with $\frac{1}{T^2}$ growing quickly as T drops, a sharp rise in specific heat.
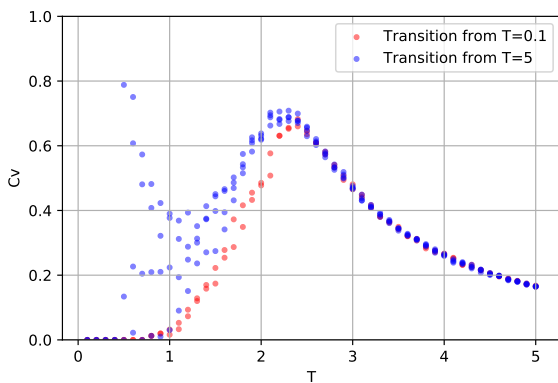

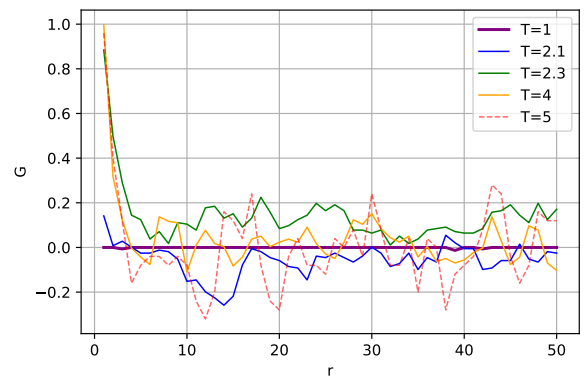Figure 6: Specific heat of spins as a function of temperature.

Figure 7: Plot of the value of the correlation function between two spins at different temperatures.

The results for the correlation function were the least conclusive, even though only the third method was used. As shown by figure 7 above, at low temperatures $G(r)$ is zero regardless of the distance - spins are uncorrelated. As T approaches the critical value, spins at increasing distances become more correlated up to T_c. At even higher temperatures, correlation decays exponentially, then fluctuates randomly around zero.

It is worth noting that an attempt was made to implement a more complex Monte Carlo method for the Ising model, namely the Wolff algorithm, which builds a whole cluster of spins based on the temperature and flips them all each loop. Even though the algorithm worked correctly, it failed to produce any relevant results due to its slowness (a consequence of its complexity) - reaching a stable state took too much time even on smaller grids.

4   Options for Further Development

The implemented model has potential for further development, as there remain quite a few relatively easily implemented features and modifications, that would allow for more in-depth exploration. These potential features are listed below.

- Find the critical exponents for the Ising model through finite size scaling.

- Add an external magnetic field and plot a hysteresis curve.

- Calculate correlation lengths for a set of temperature values, using better data for the correlation function.

- Further optimize the implemented Wolff algorithm and run the model for a longer time on a more powerful machine.

- Use a small (e.g. 2×2) grid to get analytical solutions for all calculated values and compare simulation results to theory.

5   Conclusion

The implemented Ising model, using the Metropolis-Hastings algorithm, demonstrated the expected behaviours, namely the phase transition as well as the breaking of symmetry and spontaneous magnetization below the critical temperature, which matched the analytical solution. The results for energy and specific heat met the estimations through all three used methods, while the result for spontaneous magnetization only satisfied the analytical solution through one method. It was concluded that this deviation was caused by insufficient computing power allocated to the task - the model did not have enough time to reach a truly stable state. The result for the correlation function was largely inconclusive, only roughly demonstrating the expected exponential decay of correlation between spins with distance.

References

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