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Monte Carlo Simulation of Ising Model by Python

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Abstract: Both 1D and 2D Ising model have the accurate analytical solution, this paper covers running the metropolis algorithm for the classical Ising model. Firstly, this paper discuss the simpler 1-dimensional (1D) Ising model, whose analytic solution is easier to obtain. And it calculated the magnetization, specific heat, susceptibility of a ferromagnet.

Key words: Monte Carlo; Ising model; ferromagnetism; python

Codes: python codes

1. Introduction

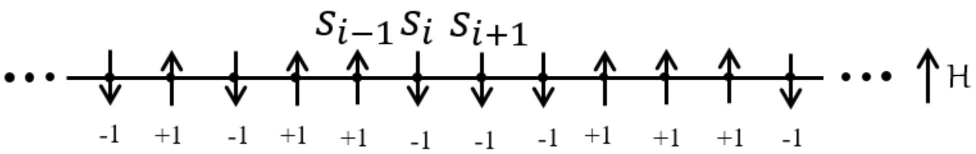
Monte Carlo simulations refer to a broad range of simulations that use a 'Pseudorandomness' approach to solve. Pseudorandomness is just a fancy way of describing statistically random numbers that are generated from something predictable, like the computer's clock.

The appeal of the Monte Carlo method is that it relies on the boundary conditions set by the user, and mimics the random statistical behavior of nature. This means complicated systems can be simulated with relatively little input.

The Ising Model is a simplified version of a ferromagnet - where the structure of the material consist of a single dipole per lattice site. The overall magnetization of the material is determined by the number of dipoles that are aligned parallel to one-another. The Ising Model is a beautifully simple detmonstration of the implications of statistical mechanics and phase transitions - as well a being an fanastic example of the power of Monte Carlo Simulations.

2. Definition of Ising model

The Ising model[1], named after the physicist Ernst Ising, is a mathematical model of erromagnetism in statistical mechanics. Ising introduced a model consisting of a lattice of “spin” variables s_i , which can only take the values +1 (↑) and −1 (↓). Every spin interacts with its nearest neighbors (2 in 1D) as well as with an external magnetic field h .



The Energy of the Ising model is[2]

$$E = -J\sum_{\langle ij\rangle} s_i s_j - \mu H \sum_i s_i \tag{1}$$

- The spins s_i can take values ± 1.
- $\langle ij \rangle$ implies nearest-neighbor interaction only.

- $J > 0$ is the strength of exchange interaction.
- H is the magnetic field and μ is the magnetic moment associated with each spin.

The Ising model is usually studied in the canonical ensemble. (It would be a nightmare to do it in the microcanonical ensemble[3]). In the canonical ensemble, the probability of finding a particular spin configuration { s_i } is

$$p(\{s_i\}) = \frac{1}{Z}\exp\left(-\beta E_{(\{s_i\})}\right) \tag{2}$$

where $Z = \sum_{\{s_i\}} \exp\left(-\beta E_{(\{s_i\})}\right)$ is the partition function. Due to the Boltzmann factor, $e^{-\beta E}$ spin configurations with lower energies will be favored.

3. 1D Ising model

The key of solving the Ising model is to get the analytical expression for partition function Z. For all the thermal parameters can be generated by partition function Z:

$$A = -k_B T \ln Z = -NJ - Nk_B T \ln\left[\cosh\beta H + \left(\sinh^2\beta H + e^{-4\beta J}\right)^{1/2}\right]$$

$$E = -\frac{\partial}{\partial\beta}\ln Z \qquad C_V = \frac{\partial E}{\partial T}$$

$$M = k_B T\frac{\partial \ln Z}{\partial H} = -\frac{\partial A}{\partial H} \qquad \chi = \frac{1}{N}\frac{\partial M}{\partial H} = -\frac{1}{N}\frac{\partial^2 A}{\partial H^2}$$

As the simplest case, Let us first consider the simpler case of $J = 0(H \neq 0)$. This is a non-interacting model.

$$Z = \sum_{\{s_i\}} \exp\left(\beta\mu H\sum_i s_i\right) = \sum_{\{s_i\}}\prod_{i=1}^{N}\exp\left(\beta\mu H s_i\right) = \prod_{i=1}^{N}\sum_{\{s_i=\pm1\}}\exp\left(\beta\mu H s_i\right)$$
$$= \left(e^{\beta\mu H} + e^{-\beta\mu H}\right)^N = \left(2\cosh\beta\mu H\right)^N$$

If we considered the interaction, It is not surprising that we will try some coordinate transformations to turn it into an equivalent non-interacting model. After all, that's all we know how to solve at this point! And we use the periodic boundary condition (PBC).

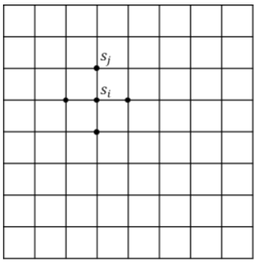
One can show that under PBC, $Z = \left(2\cosh\beta J\right)^N \cdot \left[1 + \left(\tanh\beta J\right)^N\right]$

Given the partition function Z, we can easily obtain A, E, S, M, as well as specific heat C_v .

4. 2D Ising model

4.1. Analytical solution

Consider the 2D Ising model defined over a square lattice of N spins under periodic boundary conditions. Again, the Hamiltonian can be written as



$$E = -J\sum_{\langle ij\rangle} s_i s_j - \mu H \sum_i s_i$$

J describes the strength of interaction, H is external magnetic field, and the sum $\sum_{\langle ij\rangle}$ is over all nearest neighbor pairs.Each spin has 4 nearest neighbors.

Onsager's solution in the absence of magnetic field h = 0 in the thermodynamic limit is[5]

$$A = -k_B T \ln Z \qquad Z = \lambda^N$$

$$\ln\lambda = ln\left(2\cosh 2\beta J\right) + \frac{1}{\pi}\int_0^{2\pi} dw \ln\left[\frac{1}{2}\left\{1+\left(1-K^2\sin^2 w\right)^{1/2}\right\}\right]$$

$$K = \frac{2\sin 2\beta J}{\left(\cosh 2\beta J\right)^2} \qquad \frac{k_B T_c}{J} = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.269$$

Onsager's solution predicts a phase transition at $T = T_c$.

4.2. Monte Carlo method

The Metropolis algorithm is a simple and widely used approach to generate the canonical ensemble. It is especially convenient to explain (and to implement) for an Ising model. The algorithm has the steps of [2].

The following results demonstrates the Ising model in two dimensions to calculate the energy, magnetization, specific heat and susceptibility.

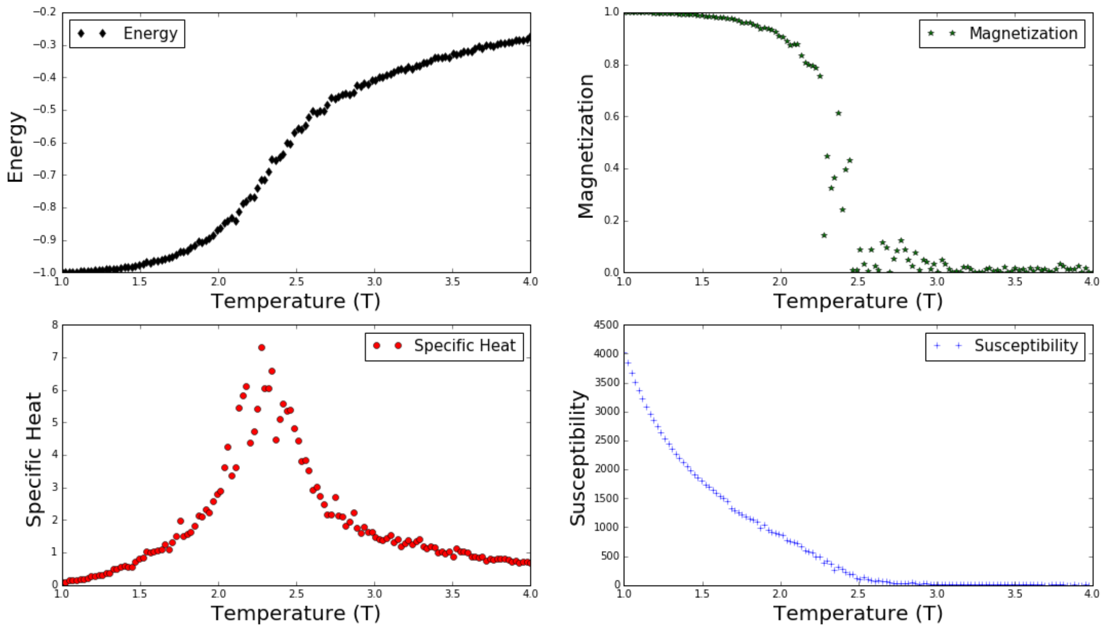


Figure 1 Energy, magnetization, specific heat and susceptibility versus temperature on a 16×16 square lattice. Here we have taken $J/k_B = 1$ and $z = 4$ corresponding to the number of nearest neighbors in a square lattice. At each temperature M was obtained by averaging over 2000 sweeps through the lattice

We can also show a dynamic evolution of a random initial configuration with specific temperature:

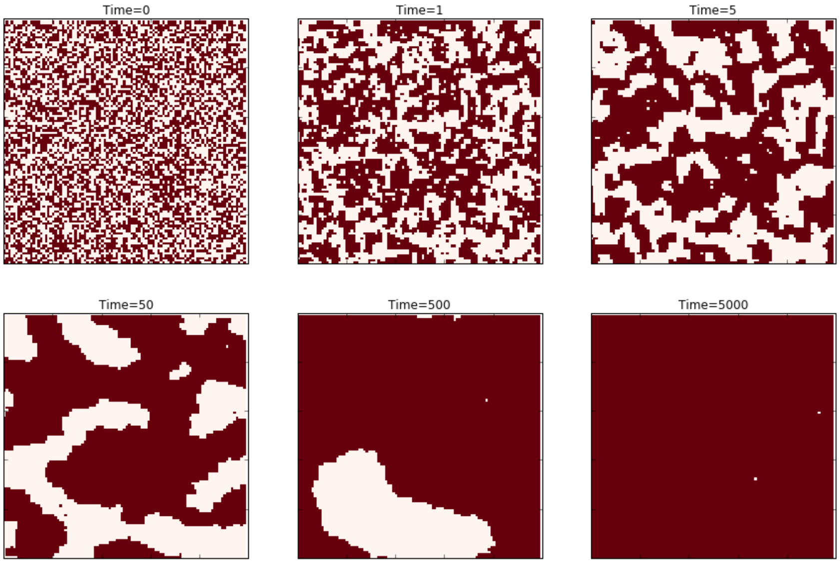


Figure 2 Snapshots of the configurations evolution versus time on a 100×100 square lattice. Here we have taken the temperature $T = 1J/k_B$, total time 5000, other parameters are the same as Figure 1.

Figure 2 shows that as the simulation progresses the interaction between the spins dominates and causes alignment. Distinct phases appear in the model. Given enough time, the system will become fully magnetized.

In comparison, this is the same simulation, but now at a high temperature limit, $T = 4J/k_B$.

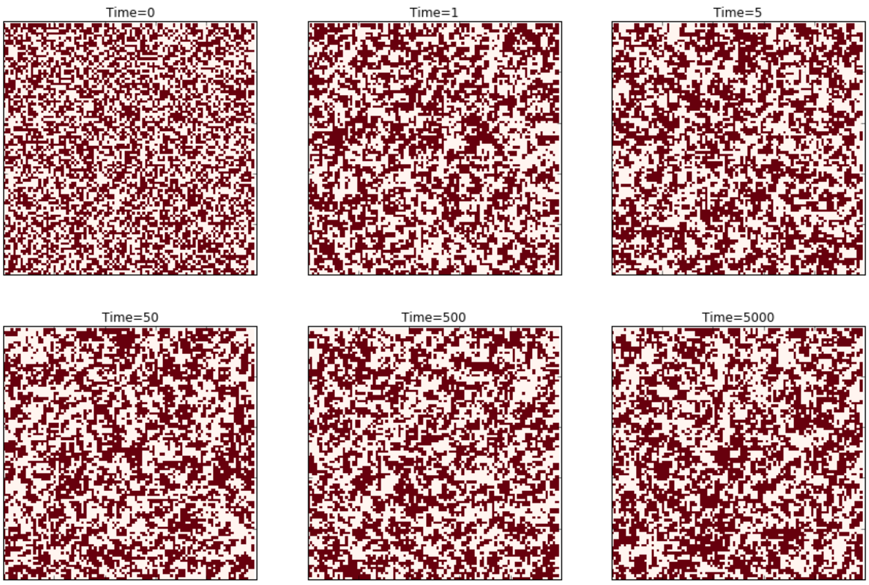


Figure 3 Snapshots of the configurations evolution versus time on a 100×100 square lattice. Here we have taken the temperature $T = 4J/k_B$.

The system remains highly disordered and the net magnetization ≈ 0.

To demonstrate the results more clearly, we plot the final configurations of different initial temperature:

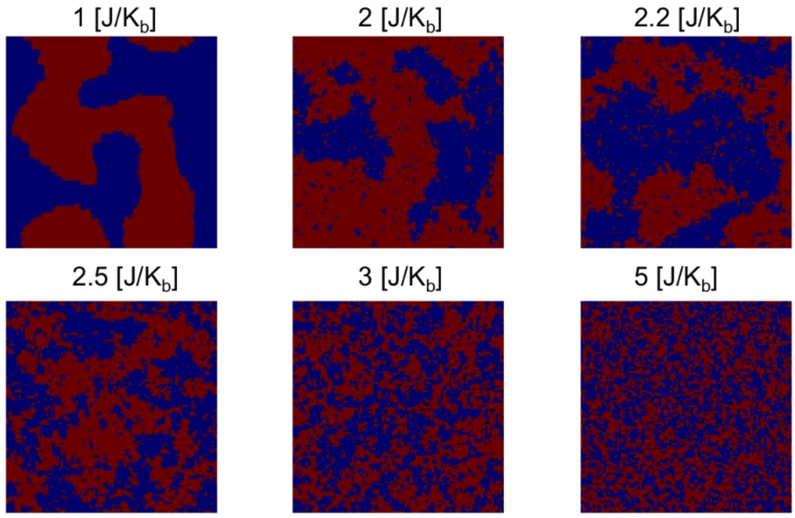


Figure 4 After enough time(t=50s), states of different temperatures. red square represent spin-up and blue square represent spin-down.

Figure 4 shows that at low temperature, that is less than $2.27 J / k_B$, there are dominances of one spin(e.g. $s_i = +1$) with fluctuations of the other spin(e.g. $s_i = -1$) as isolated clusters; numbers and size of clusters increase as temperature increase.

At critical temperature, there are no clear dominance of one spin, and the fluctuation of all scales.

At high temperature, there are no dominance of either spin, and no obvious patterns.

5. Conclusion

By utilizing the Monte Carlo method, we clearly saw that the 2D Ising model has a critical temperature T_c, below which there is spontaneous magnetization and above which there isn't. In other words, there is a phase transition at T_c.Unfortunately this doesn't occur in the 1D Ising model. The 1D Ising model does not have a phase transition.

And we find that MC method gives us that whole thermal properties of a magnetic system by calculating the partition function with statistical mechanical ideas.

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