Monte Carlo simulation of Two-dimensional Ising model

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Abstract

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1 Introduction

Ising model is a simple but important model for the explanation of magnetization. It assumes that atomic spins are located on a N-dimensional lattice grid, and these spins only have two discrete states, up ($\sigma = 1$) or down ($\sigma = -1$). Only neighboring spins can interact with each other, and thus its Hamiltonian can be written as

$$H = -J \sum_{<kl>}^{N} \sigma_k \sigma_l \,, \tag{1}$$

where $J > 0$ and $< kl >$ indicates that we only sum over nearest neighbors.

In statistical physics, the equilibrium of a system described by Eq. 1 should be solved using canonical ensemble, which involves a summation over all possible microscopic states to obtain the partition function. For N-dimensional Ising model with size L in each dimension, the total number of all microscopic states is 2^{L^N}, which cannot be simply summed over. The one- and two-dimensional cases has been solved analytically and they show several interesting properties of phase transition. But the exact solution of higher-dimensional Ising model is still unavailable, and thus numerical methods which avoid the summation over all possible states are required for the simulation of Ising model.

In this report, we discuss the Monte Carlo method for the simulation of two-dimensional (2D) Ising model and compare our results with the analytical solution. In Sec. 2 several properties shown in the analytical solution are discussed, for the comparison in Sec. 4. Sec. 3 gives the outline of Monte Carlo algorithm we utilize for 2D Ising model, and then Sec. 4 discusses the results of our simulation. Conclusions are given in Sec. 5.

2 Properties of 2D Ising model from its analytical solution

In this section we discuss the properties of $L \times L$ Ising model with periodic boundary condition, which indicates that a spin on one boundary will interact with another spin on the opposite boundary. In other words, the summation over $< kl >$ in Eq. 1 includes the following cases:

$$k = (1, x),\ l = (L, x);\ k = (x, 1),\ l = (x, L) \tag{2}$$

where (x, y) gives the coordinate of a spin in the $L \times L$ lattice.

Table 1: All possible microscopic states of 2×2 Ising model. The energy is in the unit of J.

Number of spins up	Degeneracy	Energy	Magnetization
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	-8	-4

2.1 The solution of 2×2 Ising model

For simplicity, we begin our discussion of the analytical solution from the 2×2 case. Table 1 shows all the possible microscopic states of 2×2 Ising model. The corresponding partition function can be obtained by summing over all these microscopic states α

$$Z = \sum_{\alpha} e^{-\beta E_\alpha} = 2e^{8\beta} + 2e^{-8\beta} + 12 = 4\cosh(8\beta) + 12\,, \tag{3}$$

where $\beta = 1/T$ and T is temperature in the unit of J (Boltzmann constant k_B is absorbed into T).

Thus, the mean energy of the system (in the unit of J) is

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} = -\frac{8\sinh(8\beta)}{\cosh(8\beta) + 3}\,. \tag{4}$$

The mean magnetization of the system is

$$\langle |M| \rangle = \frac{1}{Z}\sum_{\alpha} |M_\alpha| e^{-\beta E_\alpha} = \frac{1}{Z}\left(8e^{8\beta} + 4\right) = \frac{2e^{8\beta} + 1}{\cosh(8]\beta) + 3}\,. \tag{5}$$

The heat capacity is

$$C_V = \frac{\partial \langle E \rangle}{\partial T} = -\beta^2 \frac{\partial \langle E \rangle}{\partial \beta} = \beta^2 \frac{64\left[1 + \cosh(8\beta)\right]}{\left[6 + \cosh(8\beta)\right]^2} = \beta^2\left(\langle E^2 \rangle - \langle E \rangle^2\right)\,, \tag{6}$$

where

$$\langle E^2 \rangle = \frac{1}{Z}\sum_{\alpha} E_\alpha^2 e^{-\beta E_\alpha} = \frac{64\cosh(8\beta)}{\cosh(8\beta) + 3}\,. \tag{7}$$

Similarly, we have

$$\langle M^2 \rangle = \frac{1}{Z}\sum_{\alpha} M_\alpha^2 e^{-\beta E_\alpha} = \frac{8\left(e^{8\beta} + 1\right)}{\cosh(8\beta) + 3}\,, \tag{8}$$

and define susceptibility as

$$\chi = \frac{1}{\beta}\left(\langle M^2 \rangle - \langle |M| \rangle^2\right)\,. \tag{9}$$

Above results can be used to benchmark the Monte Carlo algorithm developed for 2D Ising model.

2.2 Properties of phase transition in 2D Ising model

One important aspect of the analytical solution of 2D Ising model is the phase transition at a nonzero critical temperature T_C. There is a sharp transition from nonzero $\langle|M|\rangle$ to $\langle|M|\rangle = 0$ when temperature T increases from $T < T_C$ to $T > T_C$. In this section we do not discuss the details of the analytical solution of 2D Ising model. Instead, we will show several important properties of phase transition in 2D Ising model, which are used to benchmark our simulation.

Near T_C we can characterize the behavior of many physical quantities by a power law. For 2D Ising model, the mean magnetization is given by

$$\langle M(T)\rangle \sim (T - T_C)^{\beta} \,, \tag{10}$$

where $\beta = 1/8$ is a critical exponent. A similar relation applies to heat capacity

$$C_V(T) \sim |T_C - T|^{\alpha} \,, \tag{11}$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^{\gamma} \,, \tag{12}$$

with $\alpha = 0$ and $\gamma = 7/4$. Another important quantity is called correlation length, which is expected to be of the order of the lattice spacing for $T >> T_C$. Because the spins become more and more correlated as T approaches T_C, the correlation length increases as we get closer to the critical temperature. The divergent behavior of ξ near T_C is

$$\xi(T) \sim |T_C - T|^{-\nu} \,, \tag{13}$$

with $\nu = 1$. A second-order phase transition is characterized by a correlation length which spans the whole system. Since we are always limited to a finite lattice, ξ will be proportional with the size of the lattice. Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \,, \tag{14}$$

where a is a constant and ν is defined in Eq. 13. We set $T = T_C$ and obtain a mean magnetization

$$\langle M(T)\rangle \sim (T - T_C)^{\beta} \to L^{-\beta/\nu} \,, \tag{15}$$

heat capacity

$$C_V(T) \sim |T_C - T|^{-\gamma} \to L^{\alpha/\nu}, \tag{16}$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \to L^{\gamma/\nu} \,. \tag{17}$$

The exact solution gives $\nu = 1$ and $T_C = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.269$ (in the unit of J) when $L \to \infty$. With the help of Eq. 14, we can use our simulation results of different L to extract T_C for $L \to \infty$, which will be done in Sec. 4.

3 Monte Carlo methods for Ising model

In our work the Metropolis algorithm is adopted for the simulation of Ising model. This algorithm is based on the theory of Markov chain and detailed balance. In the example of Ising model, the transition rate between two microscopic states i and j should satisfy

$$\frac{W(j \to i)}{W(i \to j)} = \frac{w_i}{w_j} = e^{-\beta(E_i - E_j)} \,, \tag{18}$$

Input: Size of the system L, temperature T, number of Monte Carlo cycles MC.
Output: $\langle E\rangle$, $\langle E^2\rangle$, $\langle|M|\rangle$, $\langle M^2\rangle$, C_V and χ.

Initialize spin lattice a (in an ordered or random way);
Calculate E, E^2, $|M|$, M^2 of the initial lattice;
$E_{tot} = 0$, $E^2_{tot} = 0$, $|M|_{tot} = 0$, $M^2_{tot} = 0$;
for $i = 1; i <= MC; i++$ **do**
    for $j = 1; j <= L; j++$ **do**
        for $k = 1; k <= L; k++$ **do**
            $r =$ a uniformly distributed random number in $[0, 1]$;
            Flip spin at position (j, k);
            Calculate the change of energy ΔE;
            if $\Delta E < 0$ or $r < \exp(-\Delta E/T)$ **then**
                Accept this spin flip;
                Update E, E^2, $|M|$, M^2;
            end
            else
                Reverse this spin flip;
            end
            Add E, E^2, $|M|$, M^2 to their corresponding "tot" variables;
        end
    end
end
Calculate the average $\langle E\rangle$, $\langle E^2\rangle$, $\langle|M|\rangle$, $\langle M^2\rangle$ by dividing L^2MC;
Calculate C_V and χ by Eq. 6 and 9;

Algorithm 1: Metropolis algorithm for the simulation of Ising model.

with $w_i = \frac{1}{Z}e^{-\beta E_i}$ to obtain an equilibrated (and detailed-balanced) probability distribution given by canonical ensemble. We can model $W(j \to i)$ as a product of the probability $T(j \to i)$ to make a transition from j to i and the probability $A(j \to i)$ to accept this transition, namely

$$W(j \to i) = T(j \to i)A(j \to i)\,. \tag{19}$$

In the simulation of Ising model, we have no physical insight of $T(j \to i)$, so we can simply assume that all $T(j \to i)$ are the same. Then Eq. 18 can be rewritten as

$$\frac{A(j \to i)}{A(i \to j)} = e^{-\beta(E_i - E_j)}\,, \tag{20}$$

which describes the probability of accepting a transition from j to i in our simulation.

Based on Eq. 20 we can develop a simulation algorithm shown in Algorithm 1. The main idea is that we flip one spin every time and use a random number r, which distributes uniformly in $[0, 1]$, to determine whether to accept this flip based on Eq. 20. If this flip reduces the energy or $r < \exp(-\Delta E/T)$ (ΔE is the energy change in the transition) we will accept. Physical quantities $\langle E\rangle$, $\langle E^2\rangle$, $\langle|M|\rangle$, $\langle M^2\rangle$ are obtained by averaging them in the Monte Carlo process.

4 Results and discussion

To be filled.

5 Conclusion

To be filled.

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References

[1] Morten Hjorth-Jensen. Overview of course material: Computational physics. `https://compphysics.github.io/ComputationalPhysicsMSU/doc/web/course`. Accessed May 4, 2018.