

Monte Carlo Simulation of Two-dimensional Ising model

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Outline

Introduction

Properties of 2D Ising model from its analytical solution

- The solution of 2×2 Ising model

- Properties of phase transition in 2D Ising model

Monte Carlo methods for Ising model

Results and discussion

- Results of 2×2 case

- Convergence and probability distribution

- Phase transition

Conclusions

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- ▶ Ising model is a simple but important model for the explanation of ferromagnetism.
- ▶ 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

$$H = -J \sum_{\langle kl \rangle}^N \sigma_k \sigma_l, \quad (1)$$

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

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- ▶ Therefore, it is necessary to develop an efficient numerical method for the simulation of Ising model.
- ▶ In this work we focus on the Monte Carlo simulation of 2D Ising model, which can be benchmarked with analytical solution.
- ▶ Our numerical framework can also be easily extended to higher dimensions.

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- ▶ We first solve 2×2 case with periodic boundary condition for benchmark.
- ▶ Periodic boundary condition: a spin on one boundary will interact with another spin on the opposite boundary.
- ▶ 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

The solution of 2×2 Ising model

- ▶ The partition function of canonical ensemble can be obtained by summing over all these microscopic states α

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

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

- ▶ The mean energy of the system (in the unit of J) is

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

The mean magnetization of the system is

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

The solution of 2×2 Ising model

- The heat capacity is

$$C_V = \frac{\partial \langle E \rangle}{\partial T} = -\beta^2 \frac{\partial \langle E \rangle}{\partial \beta} = \beta^2 \frac{64 [1 + \cosh(8\beta)]}{[6 + \cosh(8\beta)]^2}. \quad (5)$$

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- ▶ Also it can be proved that for any system under canonical ensemble

$$C_V = \beta^2 (\langle E^2 \rangle - \langle E \rangle^2), \quad (6)$$

where for 2×2 case

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

- ▶ Similarly, we have

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

and define susceptibility as

$$\chi = \beta (\langle M^2 \rangle - \langle |M| \rangle^2). \quad (9)$$

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- ▶ There is a sharp transition from nonzero $\langle |M| \rangle$ (ordered phase) to $\langle |M| \rangle = 0$ (disordered phase) when temperature T increases from $T < T_C$ to $T > T_C$.
- ▶ According to the analytical solution of 2D Ising model, the mean magnetization is given by

$$\langle M(T) \rangle \sim (T - T_C)^\beta, \quad (10)$$

where $\beta = 1/8$ is a critical exponent. Similarly heat capacity satisfies

$$C_V(T) \sim |T_C - T|^\alpha, \quad (11)$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^\gamma, \quad (12)$$

with $\alpha = 0$ (logarithmic divergence) and $\gamma = 7/4$.

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- ▶ When $T \gg T_C$, spins orient randomly without correlation, and ξ is of the order of lattice spacing.
- ▶ Spins become more and more correlated as T goes down and approaches T_C , ξ increases significantly.

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- ▶ Because we are limited to a finite lattice, ξ will be proportional with the size of the lattice when phase transition occurs.
- ▶ Through finite size scaling relation we get the critical temperature that scales as

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

where a is a constant and ν is defined in Eq. 13.

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$$\frac{W(j \rightarrow i)}{W(i \rightarrow j)} = \frac{w_i}{w_j} = e^{-\beta(E_i - E_j)}, \quad (15)$$

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$$\frac{A(j \rightarrow i)}{A(i \rightarrow j)} = e^{-\beta(E_i - E_j)}, \quad (17)$$

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

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 .

```

1 Initialize spin lattice  $a$  (in an ordered or random way);
2 Calculate  $E$ ,  $E^2$ ,  $|M|$ ,  $M^2$  of the initial lattice;
3  $E_{tot} = 0$ ,  $E_{tot}^2 = 0$ ,  $|M|_{tot} = 0$ ,  $M_{tot}^2 = 0$ ;
4 for  $i = 1; i \leq MC; i++$  do
5     for  $j = 1; j \leq L; j++$  do
6         for  $k = 1; k \leq L; k++$  do
7              $r =$  a uniformly distributed random number in  $[0, 1]$ ;
8             Flip spin at position  $(j, k)$ ;
9             Calculate the change of energy  $\Delta E$ ;
10            if  $\Delta E < 0$  or  $r < \exp(-\Delta E/T)$  then
11                Accept this spin flip;
12                Update  $E$ ,  $E^2$ ,  $|M|$ ,  $M^2$ ;
13            end
14            else
15                Reverse this spin flip;
16            end
17            Add  $E$ ,  $E^2$ ,  $|M|$ ,  $M^2$  to their corresponding "tot"
                variables;
18        end
19    end
20 end
21 Calculate  $\langle E \rangle$ ,  $\langle E^2 \rangle$ ,  $\langle |M| \rangle$ ,  $\langle M^2 \rangle$  by dividing  $L^2 MC$ ;
22 Calculate  $C_V$  and  $\chi$ ;

```

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

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Results of 2×2 case

Table 1: Results for 2×2 case with temperature $T = 1.0$. Analytical results are provided for benchmark. Energy is in the unit of J .

MC	10	100	1000	10000	Analytical
$\langle E \rangle$	-7.2	-7.92	-7.986	-7.988	-7.98393
$\langle M \rangle$	3.75	3.975	3.9955	3.99625	3.99263
$\langle E^2 \rangle$	57.6	63.36	63.888	63.904	63.8714
$\langle M^2 \rangle$	14.7	15.87	15.977	15.9805	15.9732
C_V	5.76	0.6336	0.111804	0.095856	0.128329
χ	0.6375	0.069375	0.0129798	0.0104859	0.0320873

Convergence and probability distribution

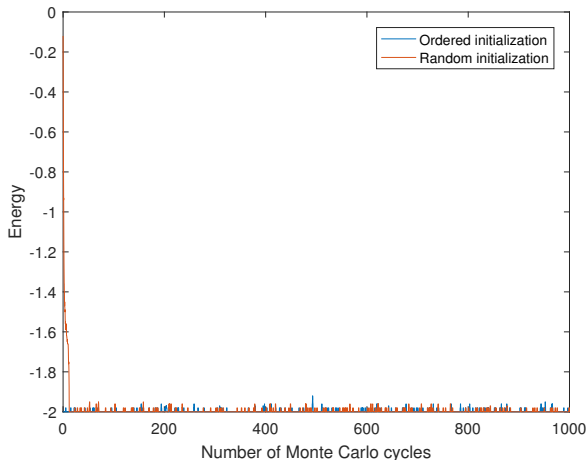


Figure 1: Energy as a function of the number of Monte Carlo cycles for $T = 1.0$, $L = 20$.

Convergence and probability distribution

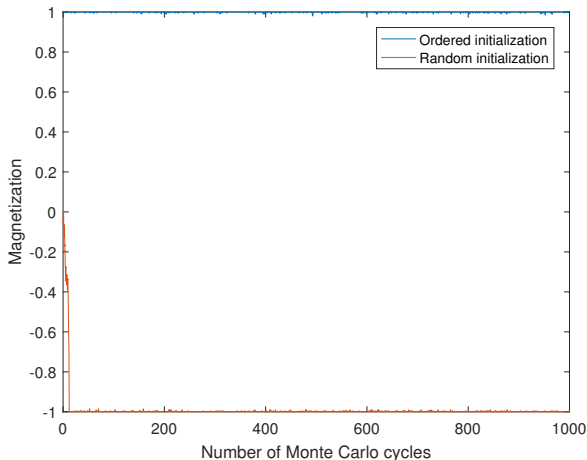


Figure 2: Magnetization as a function of the number of Monte Carlo cycles for $T = 1.0$, $L = 20$.

Convergence and probability distribution

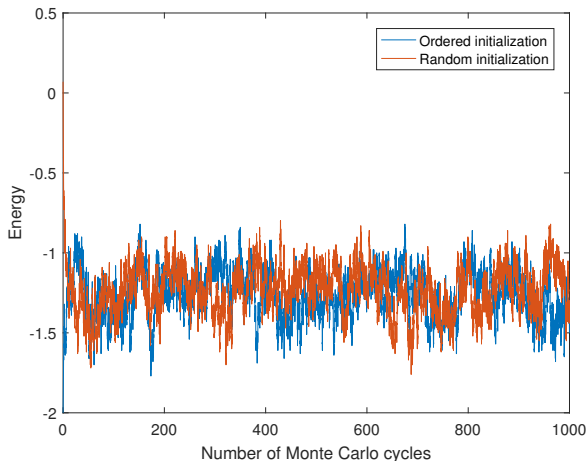


Figure 3: Energy as a function of the number of Monte Carlo cycles for $T = 2.4$, $L = 20$.

Convergence and probability distribution

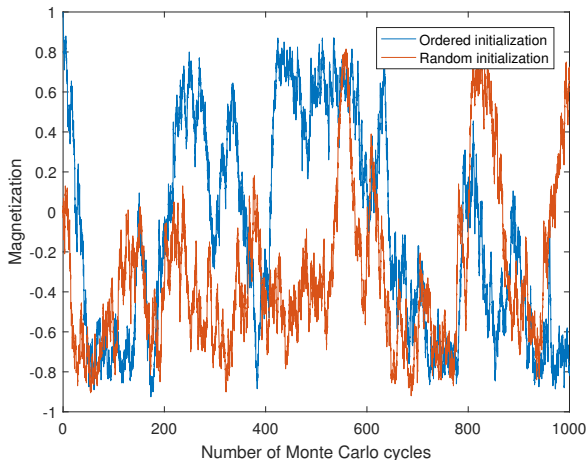


Figure 4: Magnetization as a function of the number of Monte Carlo cycles for $T = 2.4$, $L = 20$.

Convergence and probability distribution

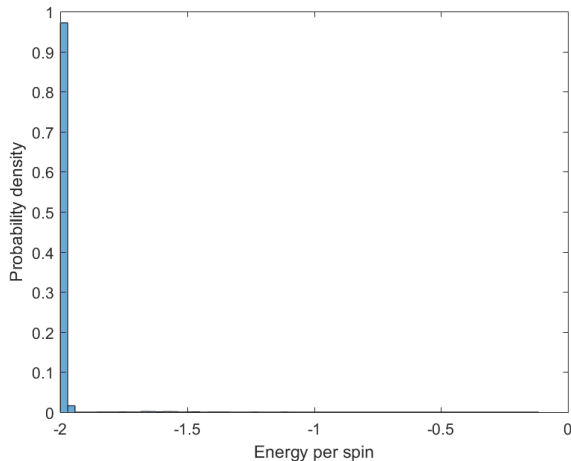


Figure 5: Distribution of energy for $T = 1.0$, $L = 20$.

Convergence and probability distribution

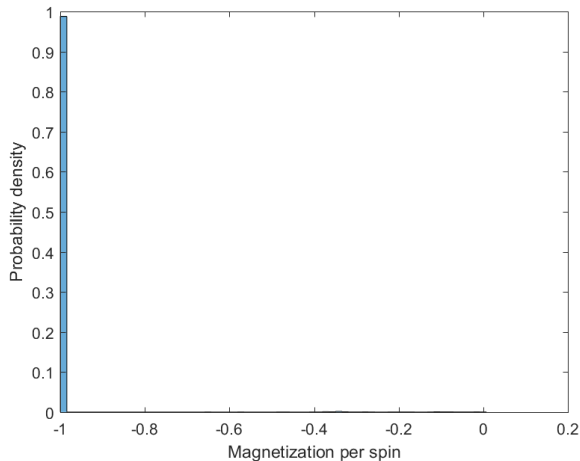


Figure 6: Distribution of magnetization for $T = 1.0$, $L = 20$.

Convergence and probability distribution

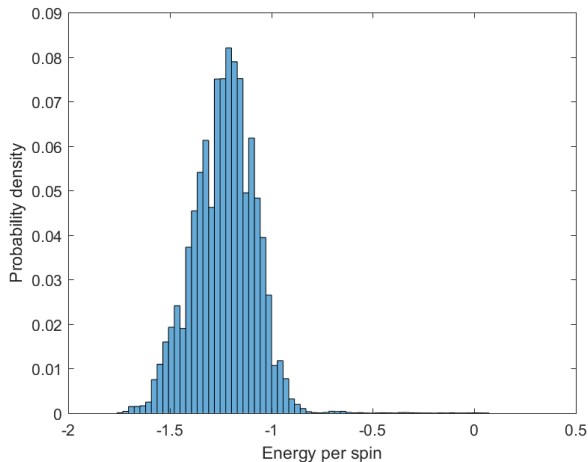


Figure 7: Distribution of energy for $T = 2.4$, $L = 20$.

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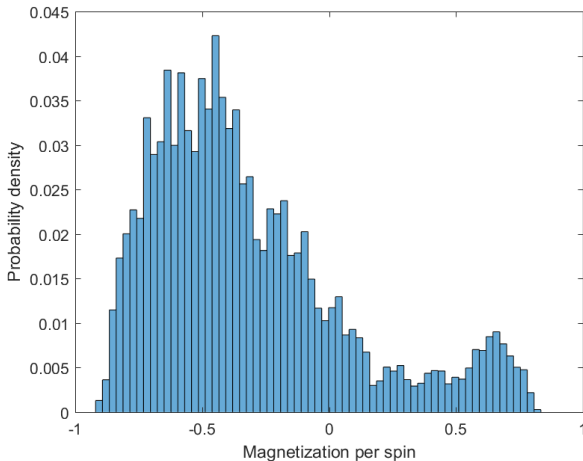


Figure 8: Distribution of magnetization for $T = 2.4$, $L = 20$.

Phase transition

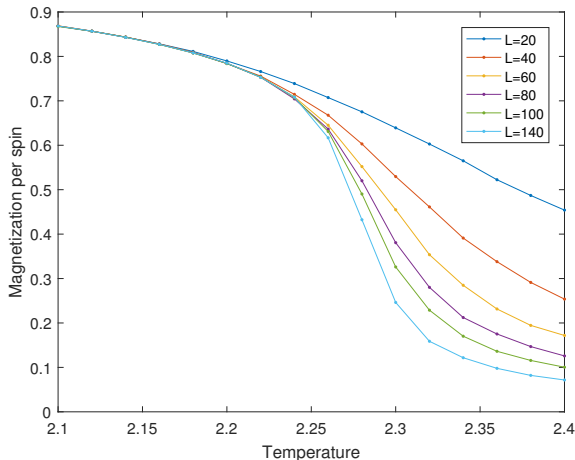


Figure 9: Magnetization per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6 .

Phase transition

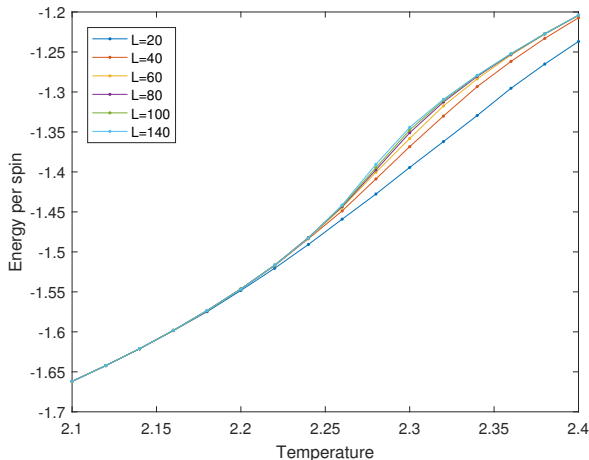


Figure 10: Energy per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6 .

Phase transition

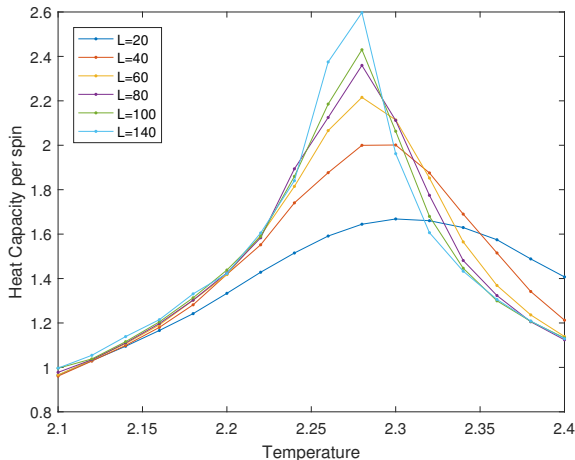


Figure 11: Heat capacity per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6 .

Phase transition

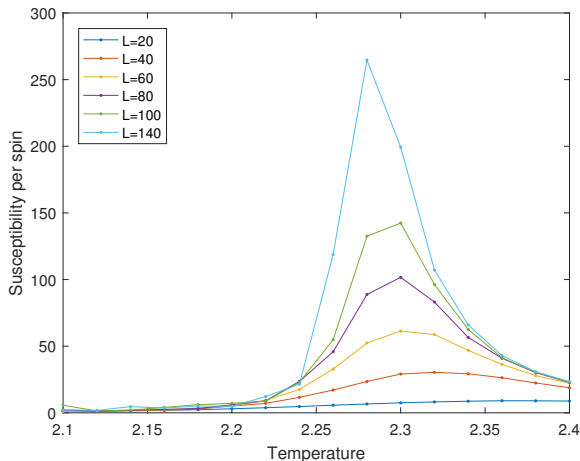


Figure 12: Susceptibility per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6 .

Estimation of critical temperature

- By the following equation

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \quad (18)$$

where a is a constant and $\nu = 1$, we can estimate T_C for an infinitely large system from the results with finite L .

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- It is quite difficult to determine the critical temperature from previous figures because our resolution is not small enough.
- From the peaks of χ we estimate that $T_C(L = 60) = 2.3$ and $T_C(L = 140) = 2.28$. Then we obtain

$$\begin{cases} a = 2.1, \\ T_C(L = \infty) = 2.265. \end{cases} \quad (19)$$

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- Our estimation is close to the analytical result 2.269.

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- ▶ In phase transition, the behaviors of different physical quantities agree well with the analytical solution.
- ▶ From the peak of susceptibility we estimate that the critical temperature for infinitely large lattice is 2.265, which is close to the analytical value 2.269.
- ▶ This work provides a powerful tool for the simulation of 2D Ising model, which can be extended to three-dimensional case.

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Thanks for your attention! Any question?