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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- 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.

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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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- 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

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

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

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- 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

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

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- The heat capacity is

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

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

$$C_V = \beta^2 \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \, , \tag{6}$$

where for 2×2 case

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

- Similarly, we have

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

and define susceptibility as

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

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- According to the analytical solution of 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. Similarly heat capacity satisfies

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

and the susceptibility

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

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

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

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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

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

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

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- $$\frac{A(j \to i)}{A(i \to j)} = e^{-\beta\left(E_i - E_j\right)}\,, \tag{17}$$

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.

```
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 ΔE < 0 or r < exp(−ΔE/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 ⟨E⟩, ⟨E^2⟩, ⟨|M|⟩, ⟨M^2⟩ by dividing L^2 MC;
Calculate C_V and χ;
```

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
$\langle \lvert M \rvert \rangle$	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

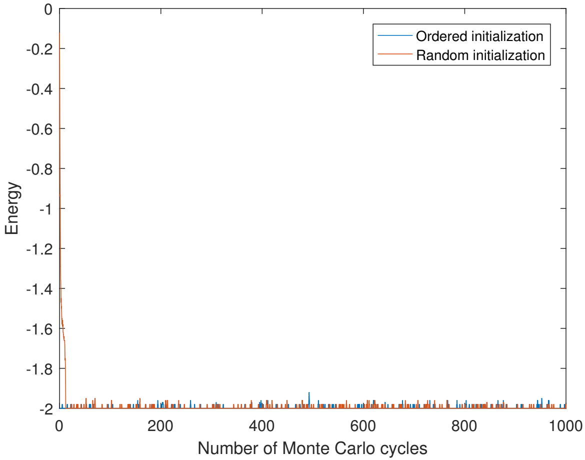

Figure 1: Energy as a function of the number of Monte Carlo cycles for $T = 1.0,\ L = 20$.

Convergence and probability distribution

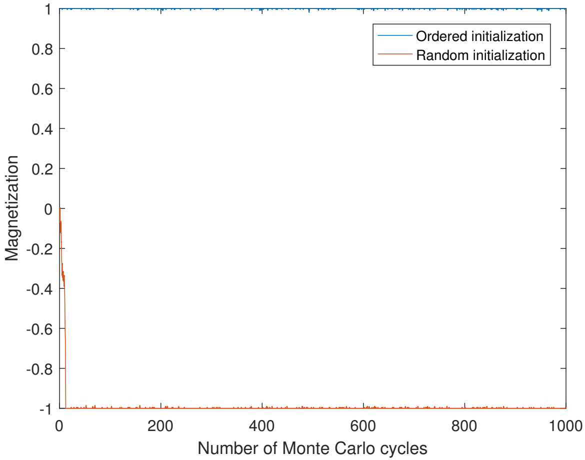

Figure 2: Magnetization as a function of the number of Monte Carlo cycles for $T = 1.0$, $L = 20$.

Convergence and probability distribution

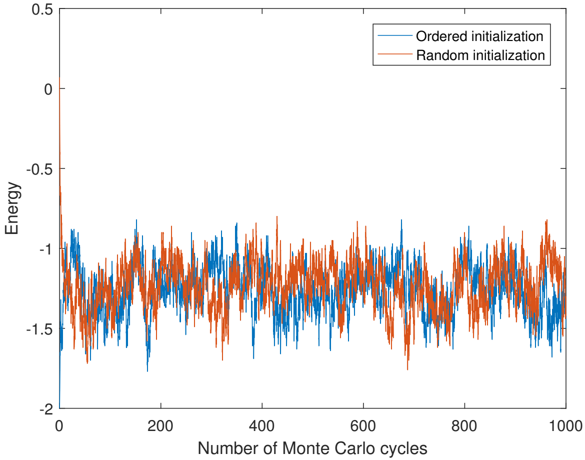

Figure 3: Energy as a function of the number of Monte Carlo cycles for $T = 2.4,\ L = 20$.

Convergence and probability distribution

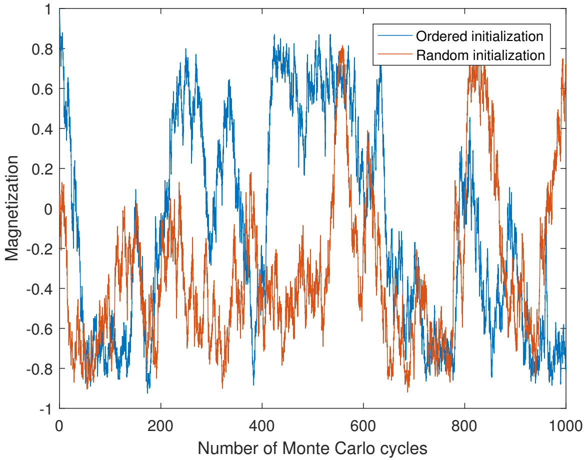

Figure 4: Magnetization as a function of the number of Monte Carlo cycles for $T = 2.4$, $L = 20$.

Convergence and probability distribution

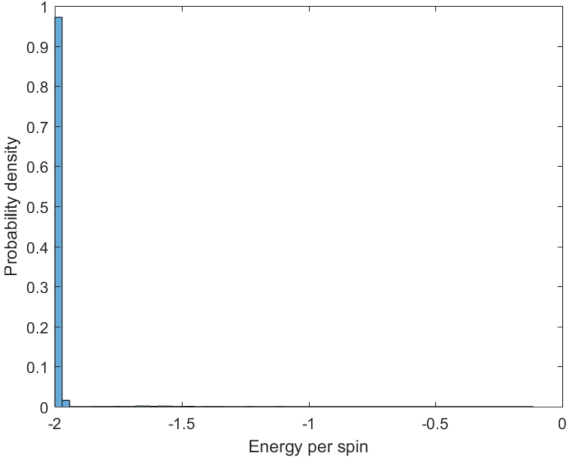

Figure 5: Distribution of energy for $T = 1.0$, $L = 20$.

Convergence and probability distribution

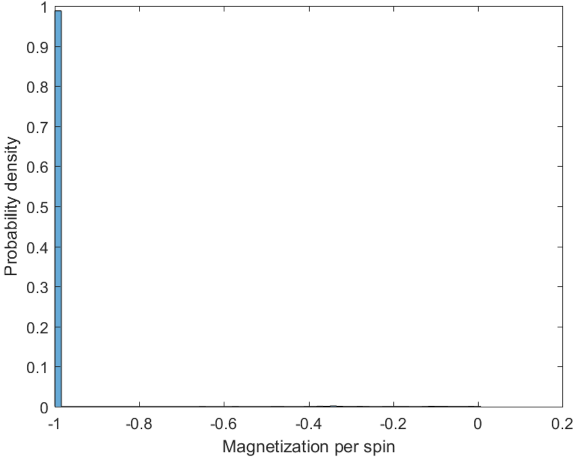

Figure 6: Distribution of magnetization for $T = 1.0$, $L = 20$.

Convergence and probability distribution

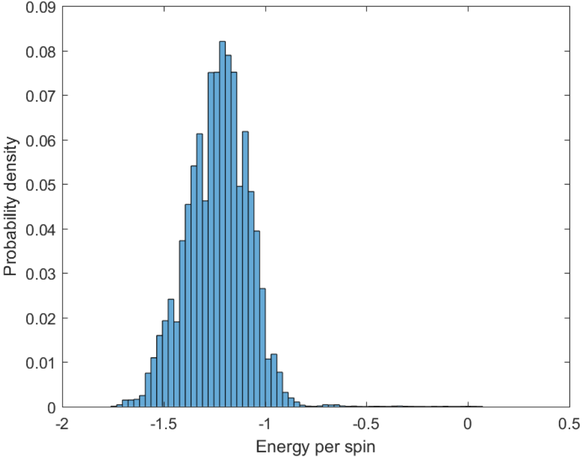

Figure 7: Distribution of energy for $T = 2.4$, $L = 20$.

Convergence and probability distribution

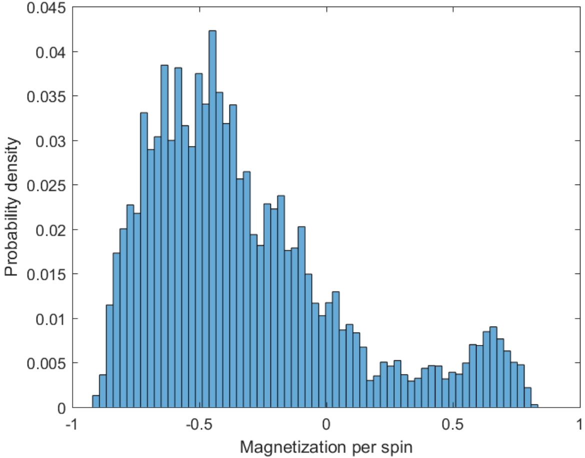

Figure 8: Distribution of magnetization for $T = 2.4$, $L = 20$.

Phase transition

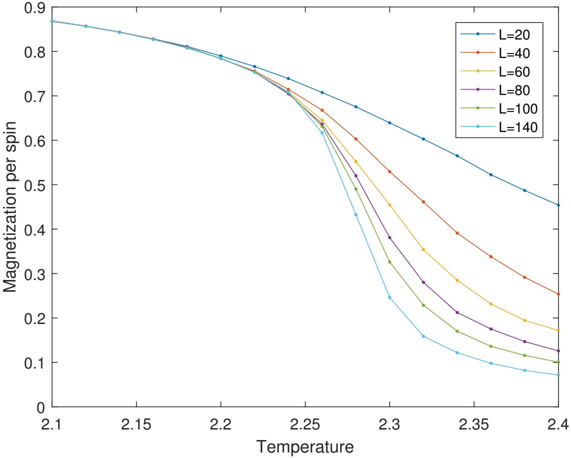

Figure 9: Magnetization per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6.

Phase transition

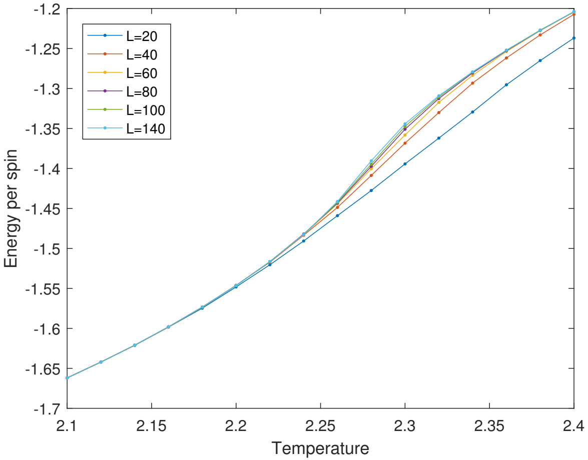

Figure 10: Energy per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6.

Phase transition

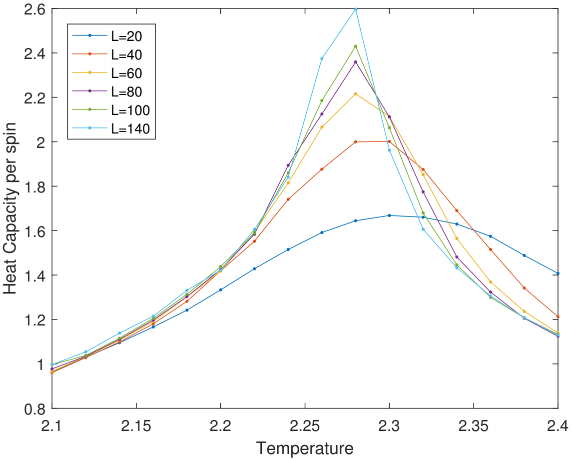

Figure 11: Heat capacity per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6.

Phase transition

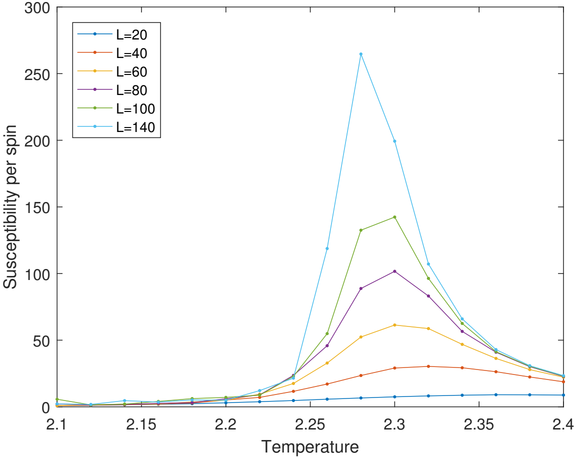

Figure 12: Susceptibility per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6.

Estimation of critical temperature

- By the following equation

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

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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- From the peaks of χ we estimate that $T_C(L=60) = 2.3$ and $T_C(L=140) = 2.28$. Then we obtain

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

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- Our estimation is close to the analytical result 2.269.

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- 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?