# Monte Carlo Simulation of Two-dimensional Ising Model


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# Outline

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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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# Properties of 2D Ising model from its analytical solution

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- We first solve $2 \times 2$ 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 $2 \times 2$ 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 $2 \times 2$ Ising model

- The partition function of canonical ensemble can be obtained by summing over all these microscopic states $\alpha$

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

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

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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

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

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- The heat capacity is

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

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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 $2 \times 2$ 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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- One interesting aspect of 2D (and higher dimensional) Ising model is the second-order phase transition at a nonzero critical temperature $T_C$.
- 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

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

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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- When $T >> T_C$, spins orient randomly without correlation, and $\xi$ is of the order of lattice spacing.
- Spins become more and more correlated as $T$ goes down and approaches $T_C$, $\xi$ increases significantly.
  The divergent behavior of $\xi$ near $T_C$ is

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  with $\nu = 1$ given by the analytical solution.
- Because we are limited to a finite lattice, $\xi$ 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 $\nu$ 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 $\chi$.

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 $\Delta E$;
            **if** $\Delta E < 0 \text{ or } r < \exp(-\Delta E/T)$ **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 $\langle E \rangle$, $\langle E^2 \rangle$, $\langle |M| \rangle$, $\langle M^2 \rangle$ by dividing $L^2 MC$;
Calculate $C_V$ and $\chi$;

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

# Outline

# Results of $2 \times 2$ case

Table 1: Results for $2 \times 2$ 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 |
| $\chi$ | 0.6375 | 0.069375 | 0.0129798 | 0.0104859 | 0.0320873 |

# Convergence and probability distribution

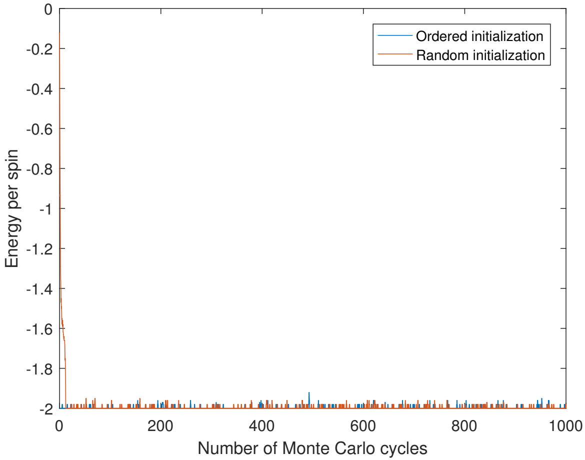


Figure 1: Energy per spin as a function of the number of Monte Carlo cycles for $T = 1.0$, $L = 20$.

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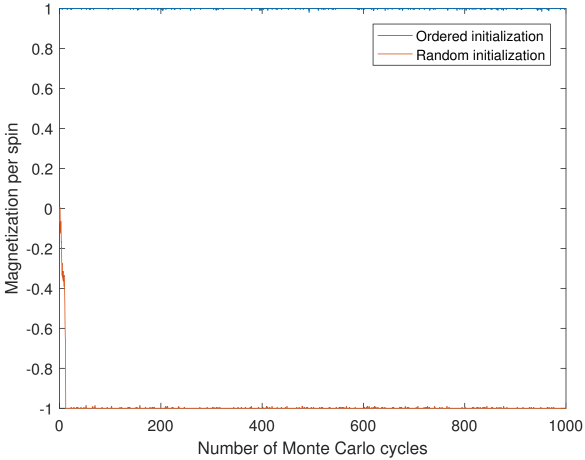


Figure 2: Magnetization per spin as a function of the number of Monte Carlo cycles for $T = 1.0$, $L = 20$.

# Convergence and probability distribution

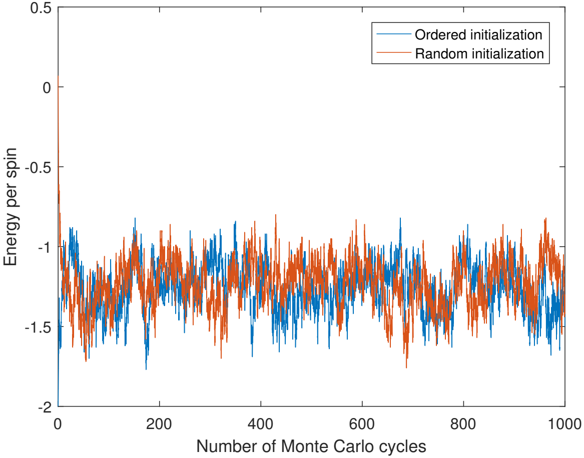


Figure 3: Energy per spin as a function of the number of Monte Carlo cycles for $T = 2.4$, $L = 20$.

# Convergence and probability distribution

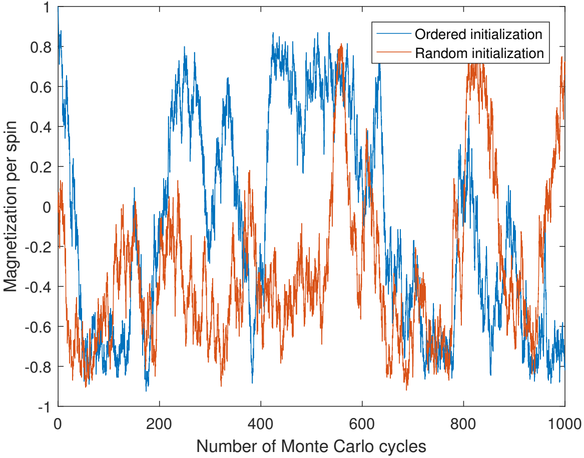


Figure 4: Magnetization per spin as a function of the number of Monte Carlo cycles for $T = 2.4$, $L = 20$.

# Convergence and probability distribution

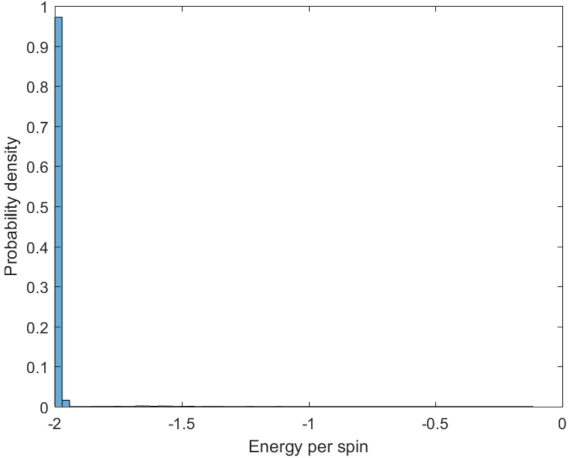


Figure 5: Distribution of energy for $T = 1.0$, $L = 20$.

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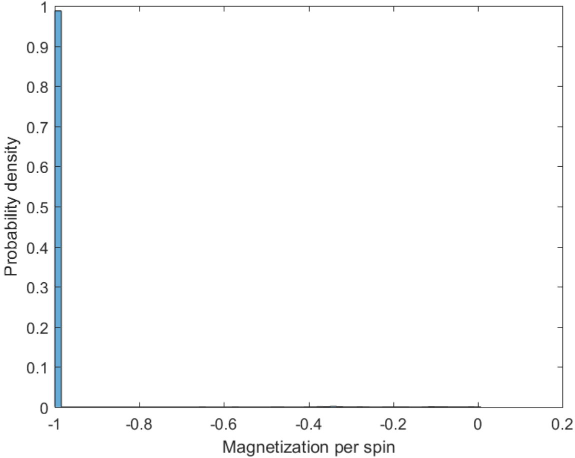


Figure 6: Distribution of magnetization for $T = 1.0$, $L = 20$.

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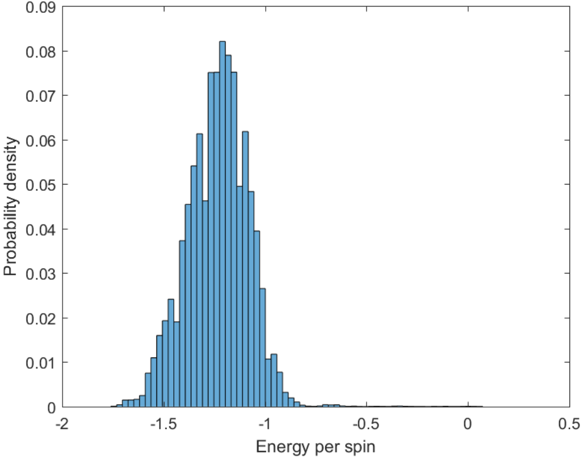


Figure 7: Distribution of energy for $T = 2.4$, $L = 20$.

# Convergence and probability distribution

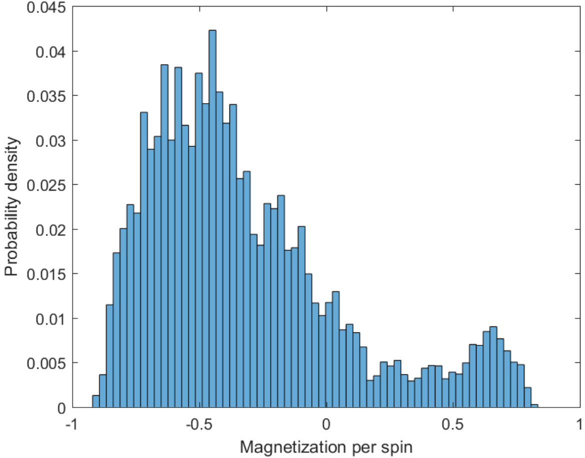


Figure 8: Distribution of magnetization for $T = 2.4$, $L = 20$.

# Phase transition

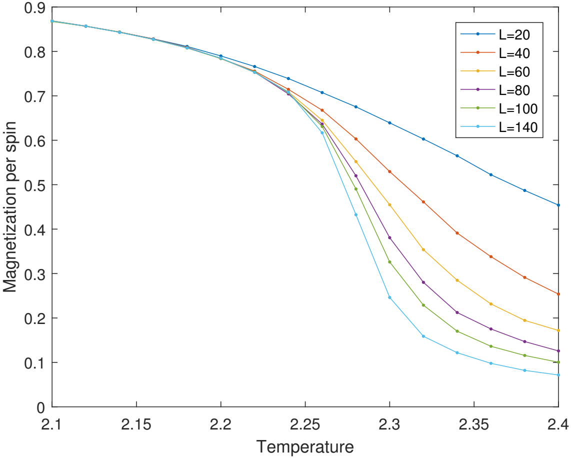


Figure 9: Magnetization per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is $10^6$.

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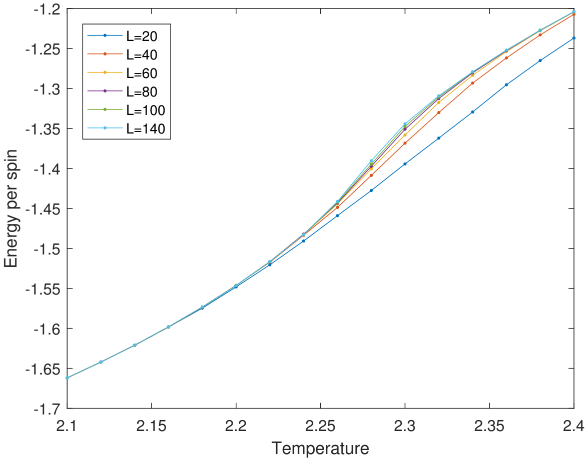


Figure 10: Energy per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is $10^6$.

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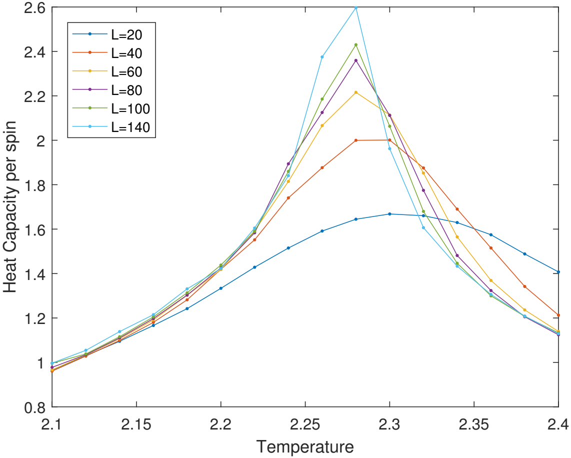


Figure 11: Heat capacity per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is $10^6$.

# Phase transition

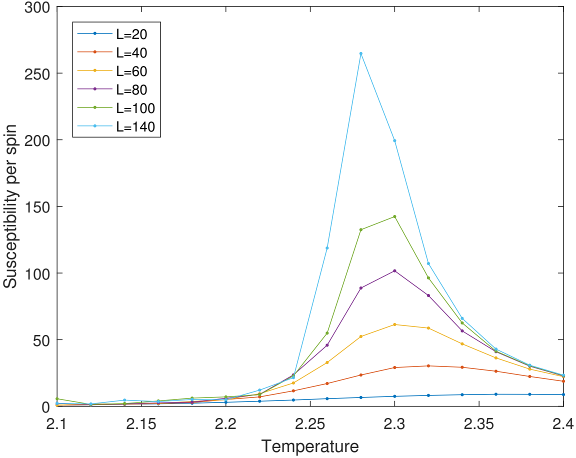


Figure 12: Susceptibility per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is $10^6$.

# 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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- It is quite difficult to determine the critical temperature from previous figures because our resolution is not small enough.
- From the peaks of $\chi$ 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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- 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?