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 ($\sigma = -1$).
- Assumption 2:
  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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- 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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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

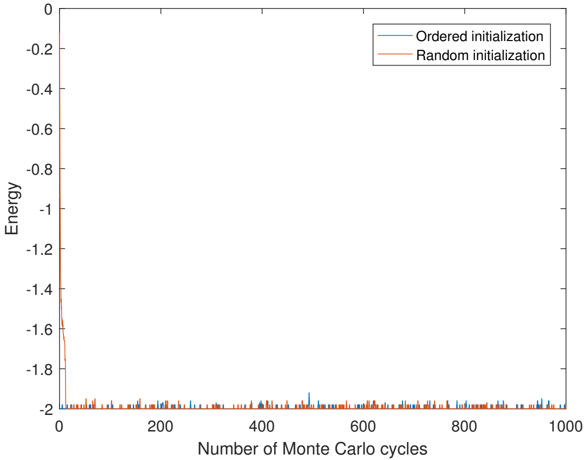

Figure 1: Energy as a function of the number of Monte Carlo cycles for $T = 1.0$, $L = 20$.

Convergence and probability distribution

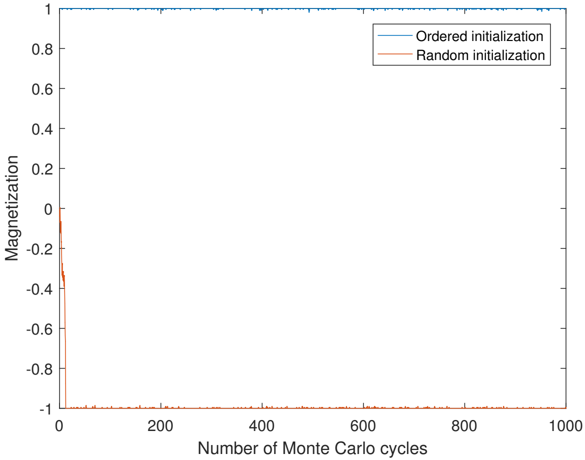

Figure 2: Magnetization as a function of the number of Monte Carlo cycles for $T = 1.0$, $L = 20$.

Convergence and probability distribution

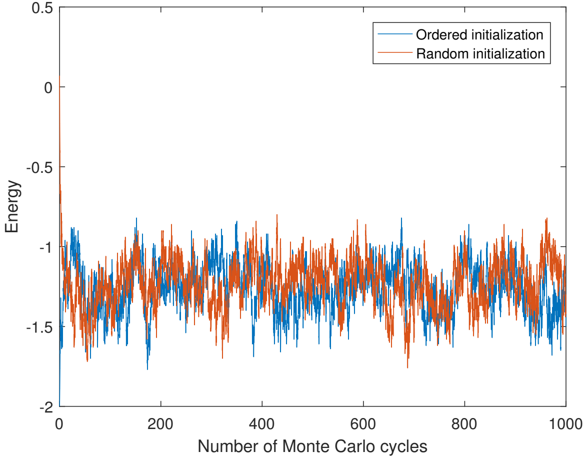

Figure 3: Energy as a function of the number of Monte Carlo cycles for $T = 2.4,\ L = 20.$

Convergence and probability distribution

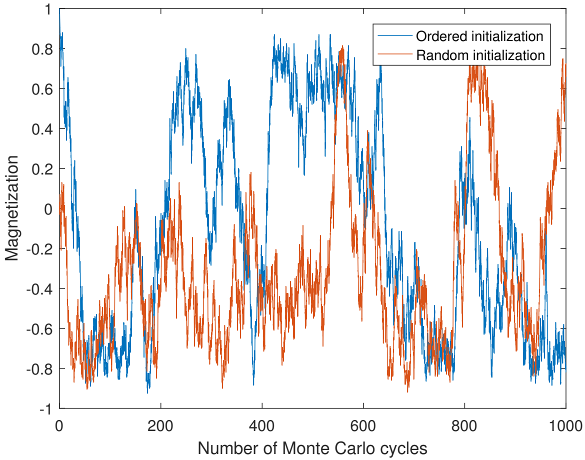

Figure 4: Magnetization as a function of the number of Monte Carlo cycles for $T = 2.4$, $L = 20$.

Convergence and probability distribution

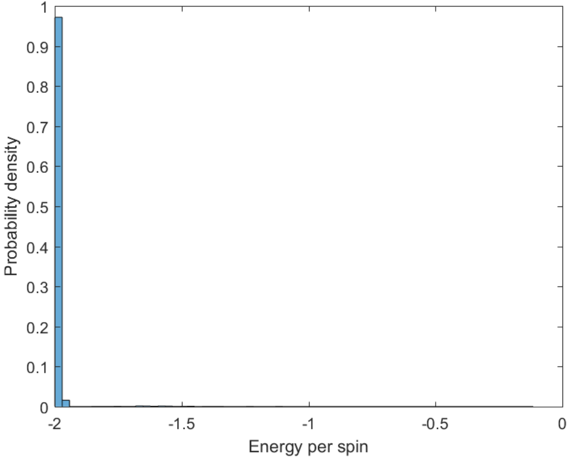

Figure 5: Distribution of energy for $T = 1.0$, $L = 20$.

Convergence and probability distribution

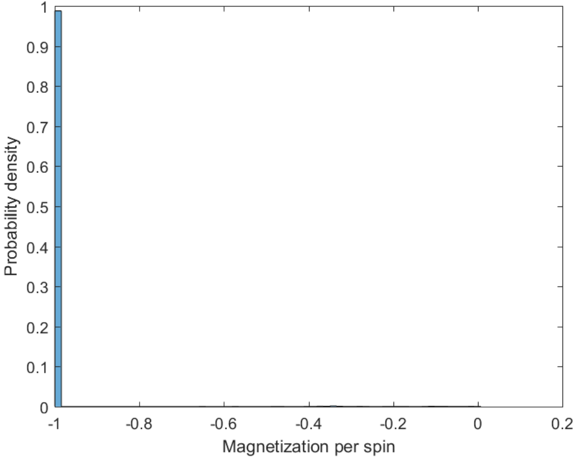

Figure 6: Distribution of magnetization for $T = 1.0$, $L = 20$.

Convergence and probability distribution

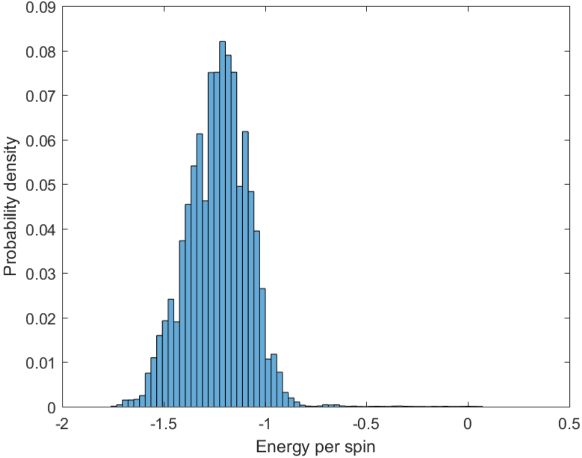

Figure 7: Distribution of energy for $T = 2.4$, $L = 20$.

Convergence and probability distribution

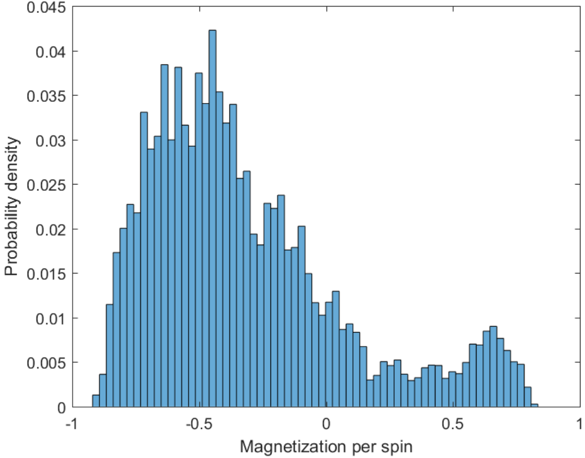

Figure 8: Distribution of magnetization for $T = 2.4$, $L = 20$.

Phase transition

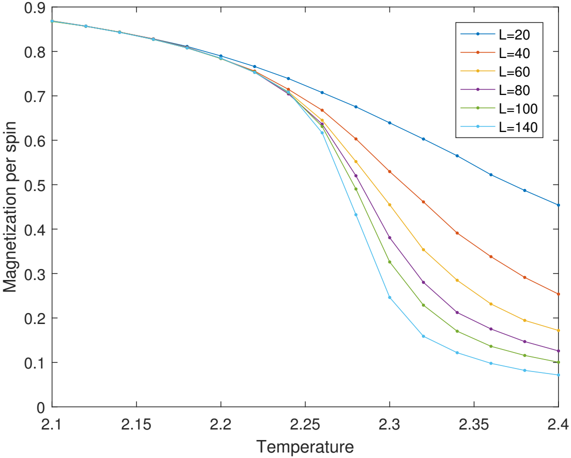

Figure 9: Magnetization per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6.

Phase transition

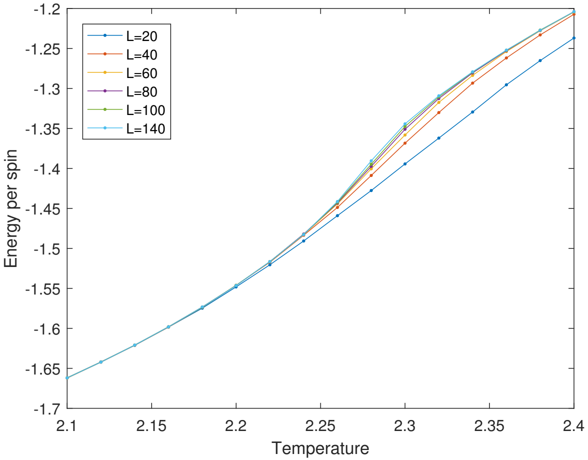

Figure 10: Energy per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6.

Phase transition

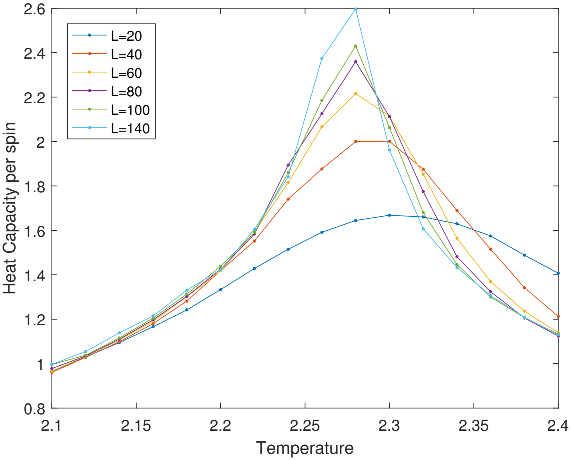

Figure 11: Heat capacity per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6.

Phase transition

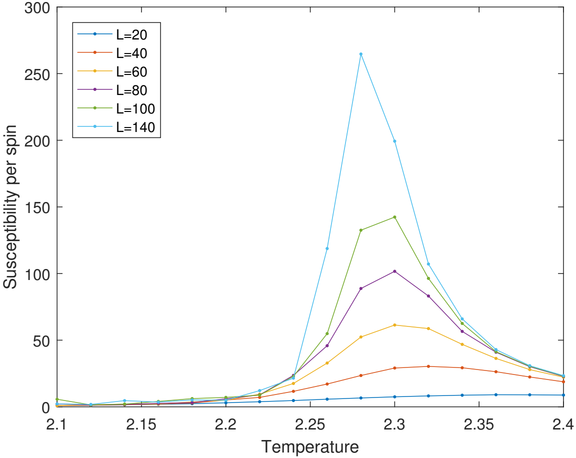

Figure 12: Susceptibility per spin as a function of temperature. Temperature step is 0.02 and the number of Monte Carlo cycles is 10^6.

Estimation of critical temperature

- By the following equation

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}\,, \tag{2}$$

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

$$\begin{cases} a = 2.1\,, \\ T_C(L = \infty) = 2.265\,. \end{cases} \tag{3}$$

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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.

Acknowledgment

I am grateful for the sincere guidance from Prof. Morten Hjorth-Jensen.

Thanks for your attention! Any question?