Critical Point of Ising Model

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Abstract

We implement the Metropolis algorithm on the 2-dimensional Ising model in order to find the critical temperature. Sicne the critical temperature can be explicitly obtained, we compare our numerical results to the theoretical results. In order to reduce error, we use large a Ising lattice and use around 10^7 sampling iteration.

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I. Settings

The 2-dimensional Ising model on the N^2 square lattice with periodic boundary condition. The Hamiltonian of the Ising model is defined as

$$H(\sigma) = -J \sum_{<i,j>} \sigma_i \sigma_j, \quad i \in [N^2]$$

where $\sigma_i = \pm 1$. We can define the following quantities:

1) Internal energy u: $u = U/N^2$, where $U =< H >$.
2) Specific heat c: $c = C/N^2$, where $C = k_B \beta^2 \mathrm{Var}(H)$

Under designated conditions, we will perform a series of numerical experiments to plot the relation $u - \beta$, $c - \beta$, find critical point $\beta^\star$. We are to adopt the traditional Metropolis-Hastings algorithm.

II. Simulation method

A. Estimate u, c

Since

$$\begin{aligned} u &= \frac{< H >}{N^2} \\ c &= k_B \beta^2 \frac{< H^2 > - < H >^2}{N^2} \end{aligned} \tag{II.1}$$

We only need to estimate $< H >, < H^2 >$.

$$\begin{aligned} < H > &\approx \frac{1}{T} \sum_{t=1}^{T} H(\sigma_t), \\ < H^2 > &\approx \frac{1}{T} \sum_{t=1}^{T} H(\sigma_t)^2 \end{aligned} \tag{II.2}$$

where σ_t is a Markov chain. It is too slow to directly calculate Hamiltonian every time we get a new stage. Instead, we update it according to the local change around the flipped spin.

B. Metropolis-Hastings Algorithm

We implemented the classical Metropolis algorithm in C++, where we construct a class named Ïsingẗo implement most operations of Ising system.

Algorithm 1 Metropolis-Hastings Algorithm

Require: J, k_B, T

$\beta = \frac{1}{k_B T}$

Initialize spins s_i within ± 1 equally randomly.

Define $H(\sigma) = -J \sum_{<i,j>} \sigma_i \sigma_j$.

repeat

  Propose a state σ'.

  Compute $\Delta H = H(\sigma') - H(\sigma_n)$, $A = \min\{1, \exp(-\beta \Delta H)\}$.

  Generate R.V. $r \sim \mathcal{U}[0, 1]$.

  If $r \leq A$, then $\sigma_{n+1} = \sigma'$; else $\sigma_{n+1} = \sigma_n$.

until convergence

III. Results

A. List of program files

1) **Ising.cpp**: critical temperature estimation of Ising model by Metropolis algorithm.
2) **Plot.m**: use data "results.csv" (generated by "Ising.cpp") to produce figures.

B. Results Presentation

We set $N = 100$ and use one Markov chain. If the β is small, we use 10^7 iterations to warm up; else, we use 5×10^8 iterations to warm up. We use 10^7 iterations to sample the results, and set $\beta = 0.1 + 0.05i$, for $i = 1, \cdots, 31$. The simulation takes about 20 min. The critical point $\beta^\star$ is around 0.45 (from file results.csv), which is close to the theoretical result $\frac{\log(1+\sqrt{2})}{2} \approx 0.44$. [Baxter, 2016]. The figure is plotted in Figure III.1.

We find that, for the temperature lower than the critical point, significantly more warming up stages are required. Especially for temperature close to zero, the probability of incurring a flip is $A \leq \exp(-\beta \Delta H) \approx 0$. Hence, the Metropolis algorithm is not efficient. There are some modifications to address the situation, such as kinetic Monte Carlo method.

References

[Baxter, 2016] Baxter, R. J. (2016). *Exactly solved models in statistical mechanics*. Elsevier.

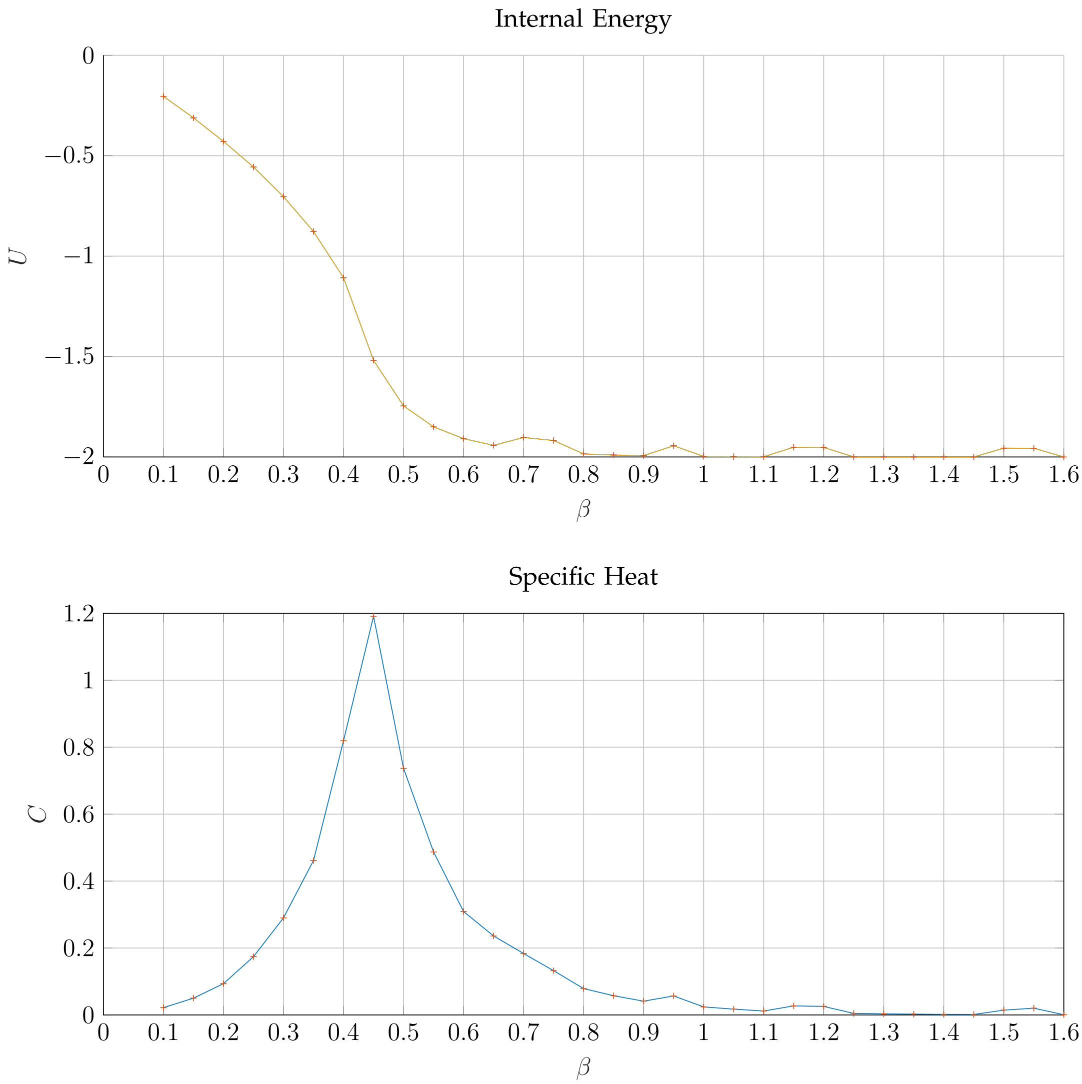

Figure III.1. Critical point: Ising model