A more concise survey on Ising model

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1 Introduction

Ising model is one of the most important model in the community of both mathematics and physics. In mathematics, it is related to various phenomena of phase transition, whose intrinsic properties remain to be justified. While in physics its importance lies in the fact that it is one of the most reliable but also simple model in atomic physics. Furthermore, the study of Ising model has generated a great many novel fields such as renormalization group theory, conformal field theory and so on. Due to the evidences listed above, deep understanding of the Ising model is highly in need. This note is some remarks and comments on a series of numerical experiments conducted on Ising model. For problem setting and derivation, please refers to the reference [1].

2 Problems in implementation

We first take a look at the energy evolution of a typical MCMC program on the Ising model. From

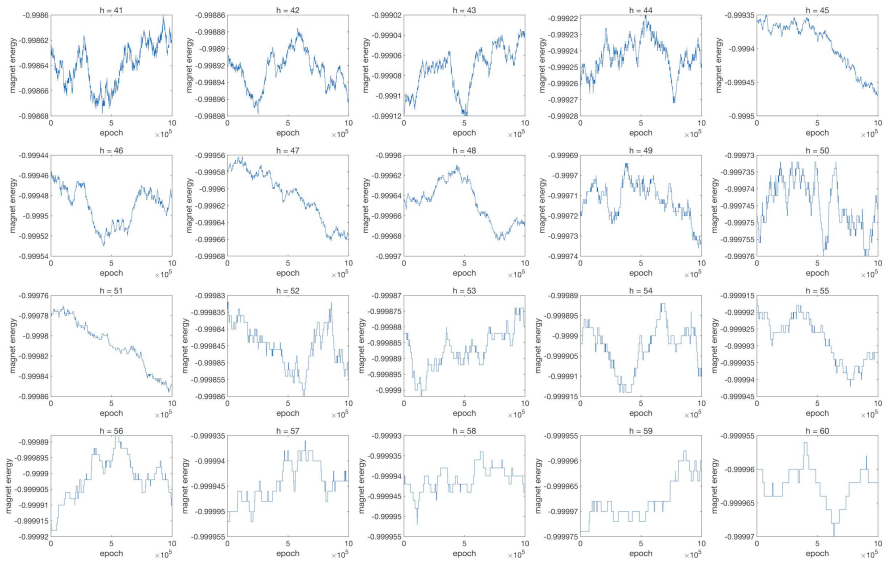

Figure 1: Energy evolution for various temperature. This figure shows the energy evolution of several simulations for different temperature

this figure, we conclude that the for most temperature, especially lower temperature, the energy of the system usually first experiences a great decrease and then it becomes oscillate. Thus, we propose a sample collecting method, which only collecting the last $10\%, 1\%$ of the sample point and compute the variance and expectation of energy according to them.

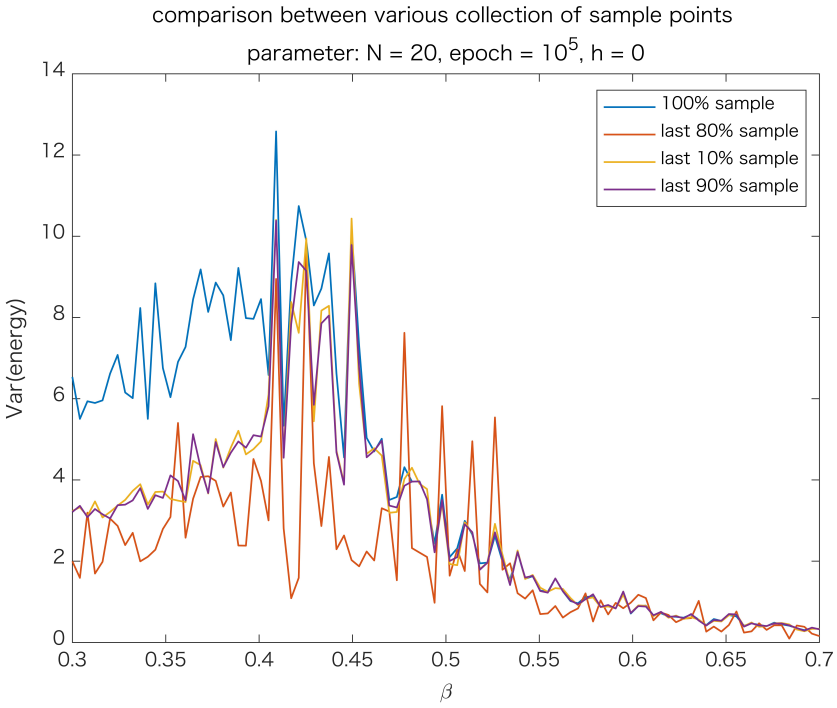

Figure 2: Comparison of different sampling. In the figure, we compare different sampling methods under the same iteration epoch and model. Convergence of the curve indicates the quality of different sampling methods.

One of the most annoying problems we faced with in implementing the MCMC on Ising model is that, although the epoch for MCMC is almost 10^8, for model with $N = 100$, the variance and average of the energy still don't converge. Specifically, the dependence between the temperature and expectation, variance of energy $\mathbb{E}_{e^{-\beta H}}[H], \mathrm{Var}_{e^{-\beta H}}(H)$ still has great many fluctuations, which is illustrated in the figure below.

To settle down this issue, we figure out several factors related to this problem.

1. Whether the size of the model, i.e. N is too big so that the MCMC cannot convergence in such a time.
2. Whether the initialization influence the result for MCMC.
3. The specific sample collecting methods influence the energy landscape.

2.1 Solution of the problems

After conducting enough numerical experiments, the most significant factor which attributes to the problem that the energy landscape w.r.t. the temperature is not smooth enough for even larger simulation epoch is eventually determined. It is various sample collecting methods that significantly influence the smoothness of the energy landscape. In this report, we show this point via plotting the energy landscapes for several choices of sample collection.

The following figure provides a description of this effect

3 Analysis of the computational complexity of MCMC on Ising model

In this section, we establish the computational complexity analysis for various methods we used to simulate on the Ising model.

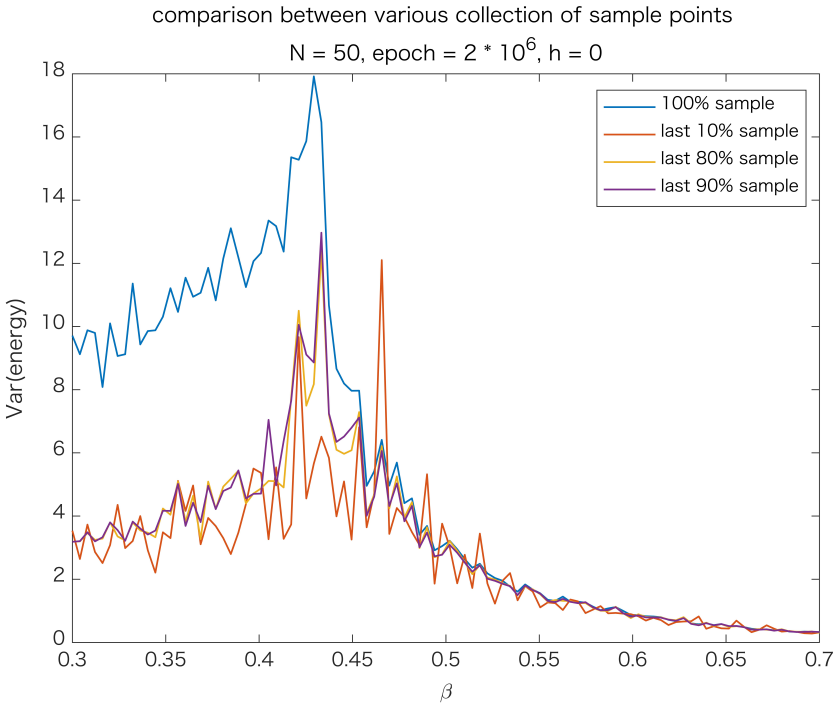

Figure 3: Comparison of different sampling

4 Conclusion

The following two figures are the result for calculating the correlation function of the Ising model [1]. Since we use the 20×20 grid to run the numerical experiment, it can be seen that correlation functions enjoy a periodic behavior with period given by 20.

5 Further Experiment

1. Accelerate the sampling of Ising model: sample 100 knots every time, so that the model get to equivalence faster, and the probability that some spins change their direction increases.

2. Try to do MCMC on 100×100 grids for computing correlation function.

3. Implement the kinetic Monte Carlo method [2] to recover above results. Here, we first discuss some implement details for realizing this algorithm. Since kinetic Monte Carlo divides all the nodes to several groups and keeps track of all the nodes and their group, it is necessary to use some efficient data structure to help us store the nodes in each group as well as sample from each group rapidly. We consider combining the C++ and Matlab programs to achieve this goal, namely, we utilize powerful data structure and operation in it in C++ and implement the whole algorithm using Matlab.

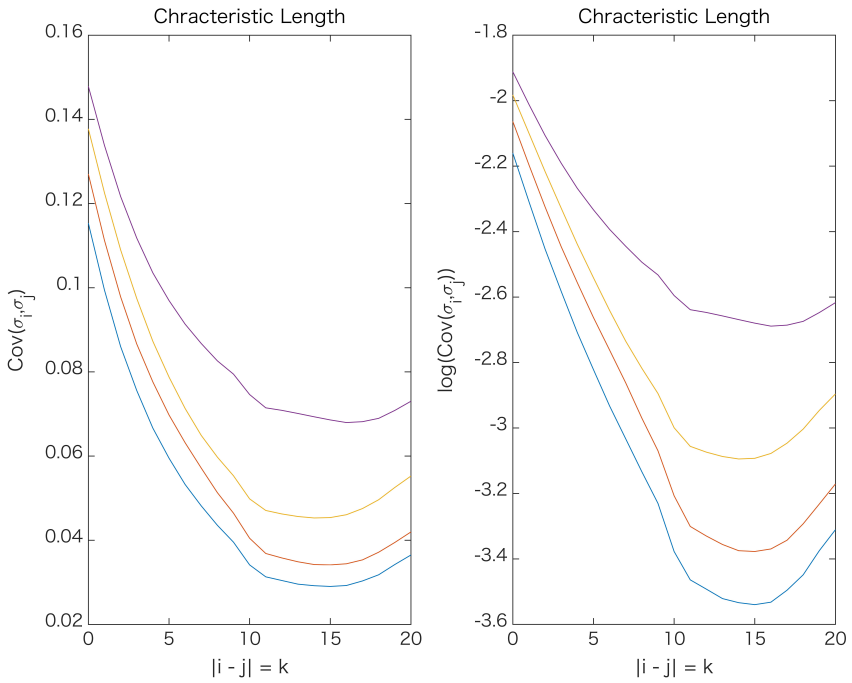

Figure 4: Correlation function with different temperatures. Different curves represent different temperatures. The lower the temperature, the lower the correlation.

References

[1] Weinan E, Tiejun Li, and Eric Vanden-Eijnden. *Applied stochastic analysis*. Graduate studies in mathematics. American Mathematical Society, Providence, RI, 2019.

[2] Arthur F. Voter. Introduction to the kinetic monte carlo method. In Kurt E. Sickafus, Eugene A. Kotomin, and Blas P. Uberuaga, editors, *Radiation Effects in Solids*, pages 1–23, Dordrecht, 2007. Springer Netherlands.

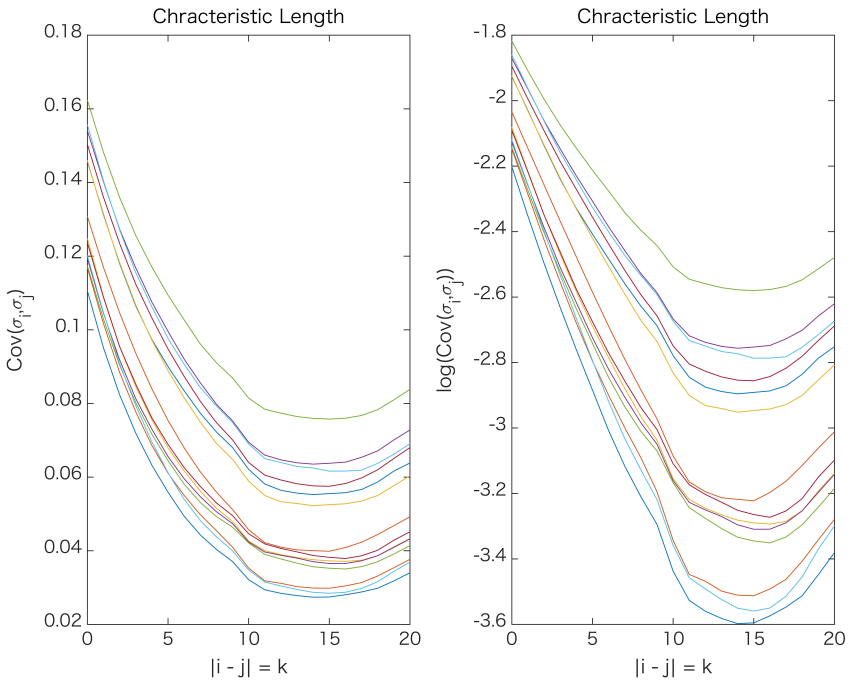

Figure 5: Correlation function with different temperatures