Markov Chain Monte Carlo Sampling and Ising Model

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1 Markov Chain Monte Carlo(MCMC) Sampling

MCMC is a Monte Carlo based method used to sample from a given distribution, $p(x)$. Here x is viewed as the state of a system, and $p(x)$ is probability that this state occurs. Jumping from one state to another state, this procedure continues for a long steps and it forms a Markov Chain. The rule guiding the state transition is a conditional probability, $p(x_{m+1}|x_m)$, which rely on the current state x_m and a possible state x_{m+1} it may jump to. This conditional probability is called *transition probability*.

MCMC is a sampling method, which means the probability of one state occurring in a Markov Chain should converge to the given distribution, $p(x)$. To achieve this goal, the Markov Chain should be *ergodicity*[1]. The ergodicity property means the Markov chain can have only one *equilibrium distribution*. A equilibrium distribution, here, refers to a distribution that is *invariant* on a Markov Chain. And a invariant distribution means the marginal distribution, $p(x_{m+1}) = \sum_{x_m} p(x_{m+1}|x_m)p(x_m)$, is not changed in a Markov Chain. A sufficient condition, for ensuring that the required distribution is invariant, is to restrain the transition probability to satisfy a property of *detailed balance*[1]. The detailed balance is defined by,

$$p(x'|x)p(x) = p(x|x')p(x')$$

The proof is,

$$\sum_s p(x'|x)p(x) = \sum_s p(x|x')p(x') = p(x') \sum_s p(x|x') = p(x')$$

If the invariant distribution is the given distribution, $p(x)$, the MCMC method can be seen as sampling from it.

2 Ising Model

The Ising model is used to describe the magnetic properties of a system. The magnetic moment of each atom of the system, s_i, is 1 or -1.

This project implement a 2D(50*50 lattice) Ising model, and use MCMC to sample from the Boltzmann distribution of the system,

$$p(x) = \frac{e^{-\beta H(x)}}{\int e^{-\beta H(x)}}$$

$$H(x) = -J \sum_{j, the\ neighbour\ of\ i} s_i s_j$$

3 Result

Let $J\beta$ =0.35, 0.55, and each runs 1000 times(1000 configurations). When $J\beta$ =0.35, each time runs 1000 Monte Carlo time steps. And when $J\beta$ =0.55, each time runs 10000 Monte Carlo steps. One Monte Carlo step contains 50*50 simulation steps. Figure 1, 2 shows the cases of $J\beta$ =0.35. Figure 3, 4 shows the cases of $J\beta$ =0.55.

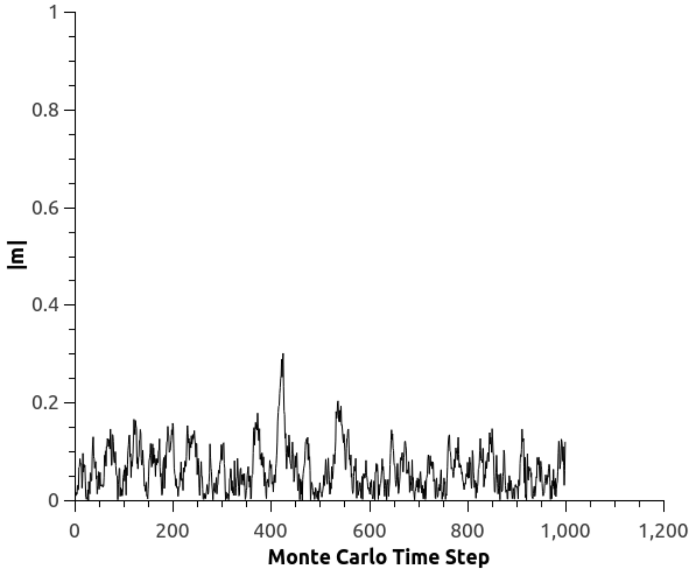

Figure 1: Ising model when $J\beta$=0.35. This is one of the 1000 configurations.

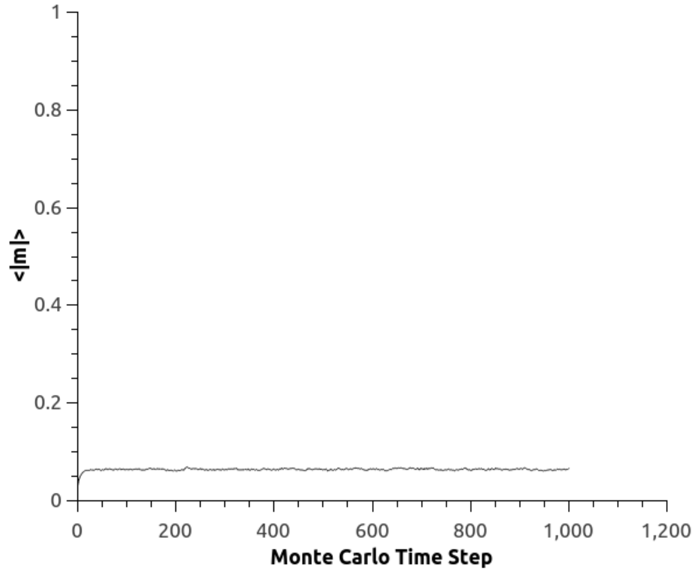

Figure 2: Ising model when $J\beta$=0.35. This is the ensemble average over 1000 configurations.

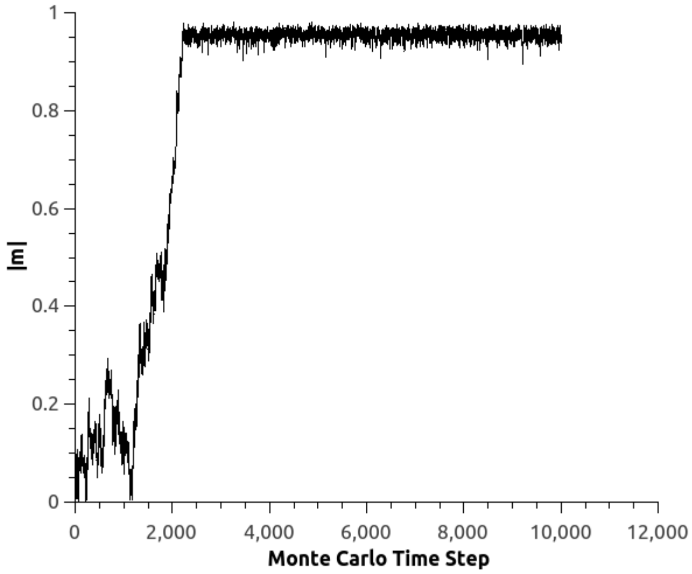

Figure 3: Ising model when $J\beta$=0.55. This is one of the 1000 configurations.

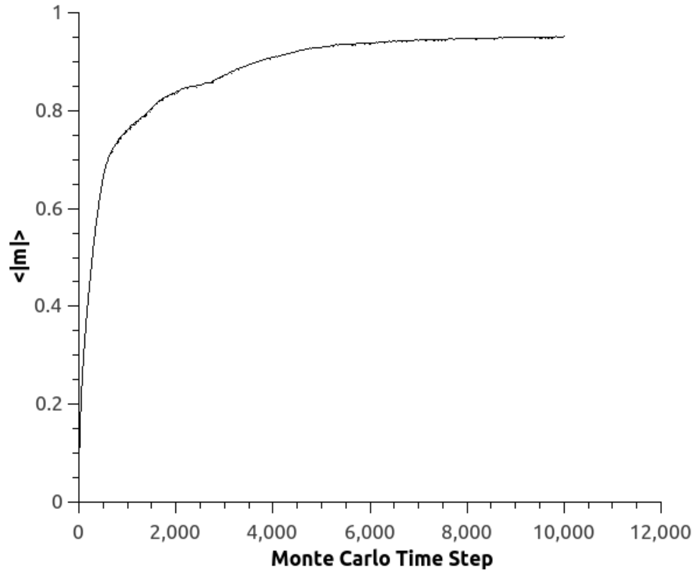

Figure 4: Ising model when $J\beta$=0.55. This is the ensemble average over 1000 configurations.

References

[1] B. Christopher, Pattern Recognition and Machine Learning, 1st ed. Springer-Verlag New York.