

Monte Carlo Simulation on Spin Glass

Week 6 Report

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I. METHODOLOGY

A. Monte Carlo simulation

The most popular and famous Monte Carlo algorithm, the Metropolis algorithm, is used to illustrate equilibration, measurement of expectation values, and the calculation of errors in a real Monte Carlo calculation. The real system is always in a subset of states with a narrow range of energies, in another word, the real system rarely makes transitions that change the energy of the system dramatically. That means, in the simulation, it is rare that the state transition change the energy of the system dramatically. With Ising Model, the simplest way of achieving this is to consider only those states which differ from the present one by the flip of a single spin, this is called *single-spin-flip dynamics*. (cite from book) The Metropolis algorithm for the Ising Model with single-spin-flip dynamics is as follows. We choose a set of selection probabilities $g(u \rightarrow v)$, one for each possible transition from one state to another, $u \rightarrow v$. Then we choose a set of acceptance probabilities $A(u \rightarrow v)$ such that a transition satisfies the condition of detailed balance, which is given by

$$\frac{P_{probability}(u \rightarrow v)}{P_{probability}(v \rightarrow u)} = \frac{p_v}{p_u} = e^{-\beta(E_v - E_u)}$$

where

- 1) p_u is given by the Boltzmann equilibrium distribution $p_u = \frac{1}{Z} e^{-\beta E_u}$.
- 2) E_u is the energy of state u .
- 3) $\beta = (kT)^{-1}$, where k is Boltzmann's constant and T is the temperature of the system.
- 4) Z is a normalizing constant, whose value is given by $Z = \sum_u e^{-\beta E_u}$.

Since in single-spin-flip dynamics, we can flip any of the N total sites,

$$g(u \rightarrow v) = \frac{1}{N}.$$

and $P_{probability}(u \rightarrow v) = g(u \rightarrow v) \cdot A(u \rightarrow v)$, plug this in to the condition of detailed balance equation. We get

$$A(u \rightarrow v) = e^{-\frac{1}{2}\beta(E_v - E_u + 2zJ)}$$

where

- 1) z is the number of neighbors that each site of the system has. On a triangular lattice structure, $z = 6$.
- 2) $2J$ is the maximum energy difference between the site we flip and its neighbors.

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Using this acceptance probability, we can correctly sample the Boltzmann distribution, however, the simulation will be very inefficient because the function $A(u \rightarrow v)$ is very small for almost all moves. This means in practice, the simulation will spend most of the time rejecting moves and not transiting to new states. Though, since the condition of detailed balance only specifies the ratio of pairs of acceptance probabilities, we can manipulate the function $A(u \rightarrow v)$ to be its optimal

$$A(u \rightarrow v) = \begin{cases} e^{-\beta(E_v - E_u)} & \text{if } E_v - E_u > 0 \\ 1 & \text{otherwise.} \end{cases}$$

The algorithm works choosing a new state v repeatedly, and then either accept or reject the new state by the acceptance probability $A(u \rightarrow v)$. If $E_v \leq E_u$, the system will always accept the transition to the new state v . Otherwise, we maybe accept it, with the probability given in the equation. If the new state is accepted, the simulated system transits to the new state v . Otherwise, the system stays as it is. This process is repeated again and again.

We start by creating a random system with a certain percentage of anti-ferromagnetic bonds.

BLAH, BLAH, BLAH...

B. Overlap

The value of overlap between two replicas, a and b , of the system is given by

$$overlap = \frac{\sum_{i=0}^N m_i^a m_i^b}{|M^a| \cdot |M^b|}$$

where

- 1) m_i^a is the average magnetization at site i in the replica a .
- 2) $|M^a| = \sqrt{\sum_{i=0}^N m_i \cdot m_i}$.

The average magnetization of site i is been calculated by adding up the spins on the site i for every 10th Monte Carlo step. Then divide by the number of spins that is been added.

C. Faces diagram

To determine which magnetic face the system is in, we consider the following two factors: the average site magnetization, m , and average of the Edwards-Anderson order parameter, $avg(\sum_i q_i)$. Edwards-Anderson order parameter is

given by $q_i = \sum_{i=0} m_i \cdot m_i$.

- 1) If $m \neq 0$ and $avg(\sum_i^n q_i) \neq 0$, the system is in the ferromagnetic face,
- 2) If $m = 0$ and $avg(\sum_i^n q_i) \neq 0$, the system is in the spin glass face, and
- 3) If $m = 0$ and $avg(\sum_i^n q_i) = 0$, the system is in the paramagnetic face.

II. PROCESS

I have ran into the wall this week dealing with the super-computer. First of all, I had trouble send and receive data between the processors. It took me a while to found the bug, which I simply passed the wrong array all the time. After fixing the communication issue, the bug that causes the value of overlap great then 1 still occurs. I found out that the value is greater than 1 only when it compares the first replica to the others. I am still in the process of debugging this issue.

However, the big improvement that I made this week was that I found a way to substitute a 2-dimension array $bond[N * N][N * N]$ with a 2-dimension array $bond[N * N][6]$. This would same a lot of the wasted memory so that I am able to run a much bigger system right now. The plan for next week is simply debugging the parallel code, and add in the features from sequential code to the parallel code.