Parallel Tempering on Monte Carlo Simulation for 2-D Ising Model

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Overview of Monte Carlo Simulation

Physical quantities follow certain distributions in some physics models. But it may be difficult to perform direct sampling because of the complexity of the state space.

Markov Chain Monte Carlo (MCMC) methods: Construct a Markov chain with desired equilibrium distribution. Running the chain will give asymptotically right estimations of physical quantities.

Underlying principle (Detailed balance): for all microstates x and y, if transition probability P(x,y) and P(y,x) satisfies:

$$\pi(x)P(x,y) = \pi(y)P(y,x)$$

The Markov chain, then, converges to an equilibrium probability distribution π at k.

Two Dimensional Ising Model

A ferromagnetism model statistical mechanics; Also useful in explaining atomic motions, thermodynamic systems and neuroscience.

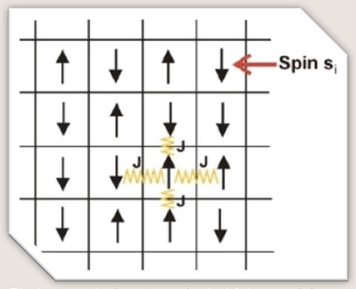

Fig 1: A particular state of a 4×4 Ising model

The model starts with a square lattice. In each position of the lattice sits an Ising spin, randomly initialized as pointing upward (magnetization +1) or downward (magnetization -1).

The total energy E and total magnetization M of the a system could be defined as follows:

$$E = -{}^{J}/_{2} \sum_{1\le i,j\le L} \sum_{(k,l)\in B(i,j)} m(i,j)m(k,l)$$

$$M = \sum_{1\le i,j\le L} m(i,j)$$

J is the interaction strength; m(i,j) is the magnetization of the spin at position (i,j), B(i,j) denotes the set of spins that are adjacent to (i,j). Periodic boundary condition is applied.

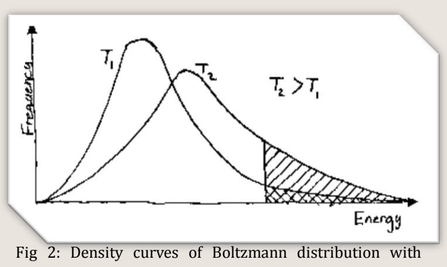

Fig 2: Density curves of Boltzmann distribution with respect to energy at different temperatures

The probability of the system at some state s at temperature T follows the Boltzmann distribution:

$$P(s;T) = \frac{\exp(-\beta E_s)}{Z(T)};\ \beta = \frac{1}{k_B T}$$

where k_B is the Boltzmann constant and Z(T) is the normalizing constant, E_s is the energy of the state.

Metropolis-Hastings Algorithm on 2-D Ising Model

Procedures for serial Metropolis algorithm:

1. Randomly generate an initial state.
2. Equilibration time, during which repeat at each step:
   i) Randomly choose a spin and propose a trail flip.
   ii) Calculate the energy difference ΔE if the flip accepted.
   iii) Accept the flip with a probability P_{flip} and otherwise retain the original microstate, where P_{flip} is given by:

$$P_{flip} = \min\{1, \exp(-\beta\Delta E)\};\ \beta = \frac{1}{k_B T}$$

3. After the equilibration, at every step we
   i) Randomly choose a spin and propose a trail flip.
   ii) Accept the flip and store the physical quantities with a probability P_{flip}.
   iii) If the flip is accepted, update the state and record energy and magnetization data.

At the end of simulation, we calculate the following physical properties of interest:

$$\text{Acceptance ratio} = \frac{\text{Number of Acceptances}}{\text{Number of Monte Carlo Steps}}$$

$$\text{Mean energy per spin} = \frac{E_{avg}}{L^2}$$

$$\text{Mean magnetization per spin} = \frac{|M|_{avg}}{L^2}$$

Parallel Tempering

Motivation: systems with low temperatures are easily trapped in "locally stable configuration", resulting in extremely low convergence rate. Note that

$$P_{flip} = \min\{1, \exp(-\beta\Delta E)\};\ \beta = \frac{1}{k_B T}$$

$$\text{As } T \to 0, \beta \to \infty, \exp(-\beta\Delta E) \to 0 \text{ for } \Delta E > 0.$$

The following shows trapped simulation in lower temperatures.

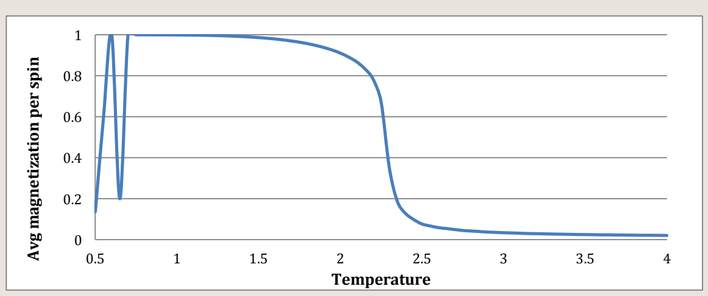

Fig 3: Results of an 80×80 Ising model with 10^9 equilibration, 10^9 Monte Carlo steps

In parallel tempering, we run several parallel systems randomly initialized. After equilibration, for every certain number of steps, configurations have a chance of being exchanged to the neighboring temperatures. The idea is to allow configurations at high temperatures to be travelled to low temperatures as the simulation process goes on, and rescue low temperature from fbeing trapped at the local minimum.

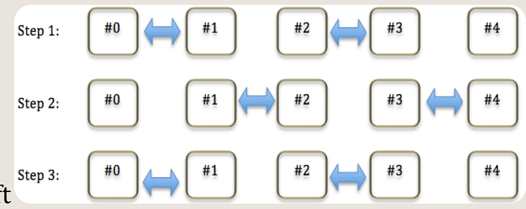

Fig 4: An illustration of exchange process in the case of five systems

For each processor, the exchange happens with its left neighbor and its right neighbor alternatively.

The acceptance probability is

$$P_{exchange} = \min\{1, \exp(\Delta\beta\delta E)\}$$

$$\Delta\beta = \beta_1 - \beta_2; \beta_i = \frac{1}{k_B T_i}$$

$$\delta E = E_1 - E_2$$

in the case of a replica exchange.

Experiment Results

The following graph shows how more frequent replica exchange will improve the convergence of simulation, particularly in lower temperatures.

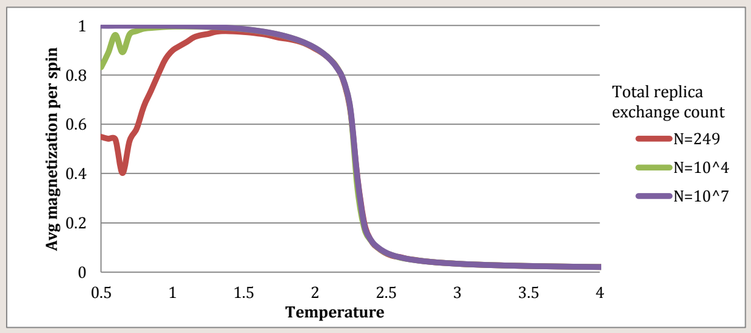

Fig 5: Results of an 80×80 Ising model with 10^9 equilibration, 10^9 Monte Carlo steps

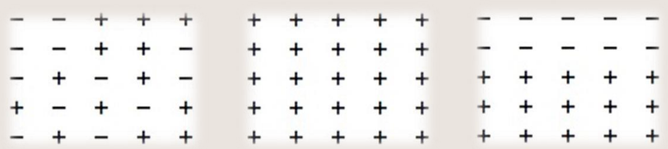
Fig 6 Illustration of three possible states in a 5*5 Ising Model

The leftmost state is more shuffled, which is more common in higher temperatures. Where the state in the middle is more ordered, and spins tend to align with each other. These states characterized by low energy are common in lower temperature. The rightmost state is a "local minimum state". It is hard to move to any other states although it is not the global energy minimum.

Simulation runs on size 80*80, with 10^9 equilibration time and MC steps, 96 processors. Temperatures are in unit of J, the interaction constant, with Botzmann constant set to 1.