Monte-Carlo Simulation

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(Advanced) Markov Chain

- Markov chain: the lack of memory of their history
- state $\{\alpha\} \rightarrow \{\beta\}$ with a transition probability $P_{\beta\alpha}$.

1. time evolution: $\rho_\beta(n+1) = \sum_\alpha P_{\beta\alpha}\rho_\alpha(n)$.
2. positivity: $0 \leq P_{\beta\alpha} \leq 1$.
3. conservation of probability: $\sum_\beta P_{\beta\alpha} = 1$.
4. not symmetric matrix: $P_{\beta\alpha} \neq P_{\alpha\beta}$.

where ρ is the probability distribution.

(Advanced) Detailed Balance

At equilibrium, they satisfy

$$P \cdot \rho^* = \rho^*,$$

where ρ^* is the equilibrium state. We introduce the condition of detailed balance as:

$$P_{\alpha\beta}\rho_\beta = P_{\beta\alpha}\rho_\alpha.$$

Then,

$$\sum_\alpha P_{\alpha\beta}\rho_\beta = \sum_\beta P_{\beta\alpha}\rho_\alpha.$$

$$\rho_\beta \sum_\alpha P_{\alpha\beta} = \sum_\beta P_{\beta\alpha}\rho_\alpha.$$

$$\rho_\beta = \sum_\beta P_{\beta\alpha}\rho_\alpha.$$

Therefore, we can arrive at the equilibrium state with the detailed balance condition.

Metropolis Algorithm

The Hamiltonian of the Ising model is

$$H = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i.$$

Then, the metropolis algorithm is following:

1. Pick a spin at random.
2. Calculate ΔE with the Ising Hamiltonian.
3. If $\Delta E < 0$, flip the spin. If $\Delta E > 0$, flip the spin with probability $e^{-\beta \Delta E}$.

[N. Metropolis et al., Equation of state calculations by fast computing machines, JCP (1953)]

Metropolis Algorithm

Check two states, 1 and 2 where $(E_1 \leq E_2)$.

$$\frac{P(1 \to 2)}{P(2 \to 1)} = \frac{\rho_1 e^{-\beta(E_2 - R_1)}}{\rho_2 \times 1}$$
$$= \frac{\rho_1 e^{-\beta E_2}}{\rho_2 e^{-\beta E_1}} = 1.$$

Due to the detailed balance, finally we have the Boltzmann distribution as

$$\rho_i \sim e^{-\beta E_i}.$$