Monte Carlo simulation

Amal Medhi

School of Physics
IISER Thiruvananthapuram

Statistical Mechanics

- Consider a system of N particles described by the Hamiltonian $\mathcal{H}$.

$$\mathcal{H} \left|s\right\rangle_n = E_n \left|s\right\rangle_n$$

- If the system where **isolated**, we would find it in any of the constant energy states $\left|s\right\rangle_n$ and the energy would be conserved.
- In practice, we often have the system in contact with a *thermal reservoir*, where there is constant exchange of energy between the system & environment.
- This gives the system a **dynamics** where the system constantly changes from one state to another.
- Since N is very large ($\sim 10^{23}$), a statistical description is only possible.

Statistical dynamics and Master equation

- Let the system be in state $|\mu\rangle$ at an instant.
- The probability that the system is in state $|\nu\rangle$ time dt later is

$$R(\mu \to \nu)dt$$

$R(\mu \to \nu)$ is called the **transition rate** (assumed time independent).

Statistical dynamics and Master equation

- Let the system be in state $|\mu\rangle$ at an instant.
- The probability that the system is in state $|\nu\rangle$ time dt later is

$$R(\mu \to \nu)dt$$

  $R(\mu \to \nu)$ is called the **transition rate** (assumed time independent).
- So if we start with the system in state $|\mu\rangle$, it can transition to any other possible state after a short time.
- We can define a set of weights $w_\mu(t)$ which represent the probability that the system is in state $|\mu\rangle$ at time t.
- The master equation defines the evolution of these weights,

$$\frac{dw_\mu(t)}{dt} = \sum_\nu [w_\nu(t)R(\nu \to \mu) - w_\mu(t)R(\mu \to \nu)]$$

- We must have $\sum_\mu w_\mu(t) = 1$.

Statistical Mechanics

- **Expectation value:** For a physical observable A,

$$\langle A \rangle = \sum_{\mu} A_{\mu} w_{\mu}(t)$$

Statistical Mechanics

- **Expectation value:** For a physical observable A,

$$\langle A \rangle = \sum_{\mu} A_{\mu} w_{\mu}(t)$$

- **Equilibrium:** If the rhs of the master equation vansihes, then the weight $w_{\mu}(t)$ will become constant.
- For any system obeying master equation, it is bound to happen as $t \to \infty$ (because $0 \leq w_m u(t) \leq 1$ and $w_m u(t)$ can not grow infinitely).
- Define equilibrium probability distribution,

$$p_{\mu} = \lim_{t \to \infty} w_{\mu}(t)$$

Statistical Mechanics

- **Expectation value:** For a physical observable A,

$$\langle A \rangle = \sum_{\mu} A_{\mu} w_{\mu}(t)$$

- **Equilibrium:** If the rhs of the master equation vansihes, then the weight $w_{\mu}(t)$ will become constant.
- For any system obeying master equation, it is bound to happen as $t \rightarrow \infty$ (because $0 \leq w_m u(t) \leq 1$ and $w_m u(t)$ can not grow infinitely).
- Define equilibrium probability distribution,

$$p_{\mu} = \lim_{t \rightarrow \infty} w_{\mu}(t)$$

- For a system in thermal equilibrium at T, we know that

$$p_{\mu} = \frac{1}{Z} e^{-\beta E_{\mu}}$$

- Z is the partition function, $Z = \sum_{\mu} e^{-\beta E_{\mu}}$.

Ising Model

- Consider the **Ising model** in statistical physics

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j$$

- $S_i = \pm 1$ are classical spin variables. The sum is over nearest neighbour sites $\langle i, j \rangle$.

Ising Model

- Consider the **Ising model** in statistical physics

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j$$

- $S_i = \pm 1$ are classical spin variables. The sum is over nearest neighbour sites $\langle i, j \rangle$.
- For $J > 0$, the ground state will have all spins aligned. **Ferromagnetic order**.
- At temperature $T > 0$, there will be thermal fluctuation. At $T = T_c$, there is a phase transition to paramagnetic state.

Ising Model

- Consider the **Ising model** in statistical physics

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j$$

- $S_i = \pm 1$ are classical spin variables. The sum is over nearest neighbour sites $\langle i, j \rangle$.
- For $J > 0$, the ground state will have all spins aligned. **Ferromagnetic order**.
- At temperature $T > 0$, there will be thermal fluctuation. At $T = T_c$, there is a phase transition to paramagnetic state.
- We need to calculate the expectation values,

$$\langle A \rangle = \frac{1}{Z} \sum_{\mu} A_\mu e^{-\beta E_\mu}$$

- The sum is over the states $|\mu\rangle$. An example state for a 4 sites lattice is

$$|\mu\rangle = |+1,\ -1,\ -1,\ +1\rangle$$

Ising Model

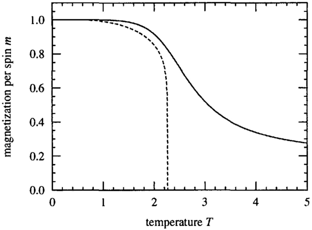
Problem of large numbers

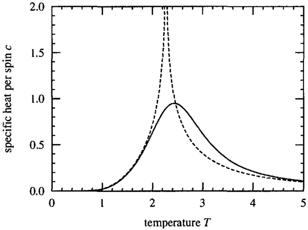
- The total number of possible states of the Ising model is $N = 2^L$, L is the number of sites.
- Suppose we want to carry out the sum exacty in a computer.
- If we take a 5×5 lattice, we have to sum over $N = 2^{25} = 33,554,432$ states. Not a small number.
- If we increase the size to 6×6, we would have 2048 times more states!

Ising Model

Problem of large numbers

- The total number of possible states of the Ising model is $N = 2^L$, L is the number of sites.
- Suppose we want to carry out the sum exacty in a computer.
- If we take a 5×5 lattice, we have to sum over $N = 2^{25} = 33,554,432$ states. Not a small number.
- If we increase the size to 6×6, we would have 2048 times more states!
- And we need take **large** lattice in order to capture the real physics. Example: studying phase transition of the 2D Ising model for 5×5 lattice:





Monte Carlo simulation

- The main problem here is the evaluation of the following average,

$$\langle A \rangle = \frac{1}{Z} \sum_{\mu} A_{\mu} e^{-\beta E_{\mu}}$$

- For large L, it is impossible to evaluate the exact sum.

Monte Carlo simulation

- The main problem here is the evaluation of the following average,

$$\langle A \rangle = \frac{1}{Z} \sum_{\mu} A_{\mu} e^{-\beta E_{\mu}}$$

- For large L, it is impossible to evaluate the exact sum.
- Monte Carlo work by choosing only a subset of states randomly for evaluating the sum.
- Let this subset by $\{\mu_1, \mu_2, \ldots, \mu_M\}$, where $M \ll N = 2^L$.
- Suppose these states are generated from a particular probability distribution p_{μ}.
- Then the best estimate for the quantity $\langle A \rangle$ would be,

$$\overline{A}_M = \frac{\sum_{i=1}^{M} A_{\mu_i} p_{\mu_i}^{-1} e^{-\beta E_{\mu_i}}}{\sum_{i=1}^{M} p_{\mu_i}^{-1} e^{-\beta E_{\mu_i}}}$$

- $\overline{A}_M$ is called an estimator of $\langle A \rangle$. We expect: $\lim_{M \to \infty} \overline{A}_M = \langle M \rangle$.

Monte Carlo simulation

- **Importance sampling**: If we choose the states with a probability distribution equal to their Boltzmann weight, that is $p_\mu = e^{-\beta E_\mu}/Z$, then

$$\overline{A}_M = \frac{1}{M}\sum_{i=1}^{M} A_{\mu_i}$$

- This is analogous to what a *real system* would go through. Though it has a large number of accessible states, it spend most of the time in only fraction of important states determined by the Boltzmann factor.

Monte Carlo simulation

- **Importance sampling**: If we choose the states with a probability distribution equal to their Boltzmann weight, that is $p_\mu = e^{-\beta E_\mu}/Z$, then

$$\overline{A}_M = \frac{1}{M} \sum_{i=1}^{M} A_{\mu_i}$$

- This is analogous to what a *real system* would go through. Though it has a large number of accessible states, it spend most of the time in only fraction of important states determined by the Boltzmann factor.
- The question is how to choose a subset of states from the probability distribution $p_\mu = e^{-\beta E_\mu}$?

Markov process

- Suppose we start with a state $|\mu\rangle$. Next we generate a state $|\nu\rangle$ randomly. Probability of going to ν from μ is called the **transition probability** $W(\mu \to \nu)$. For a Markov process, it must satisfy two conditions
  - $W(\mu \to \nu)$ should not vary over time.
  - $W(\mu \to \nu)$ depend only upon $|\mu\rangle$ and $|\nu\rangle$.

Markov process

- Suppose we start with a state $|\mu\rangle$. Next we generate a state $|\nu\rangle$ randomly. Probability of going to ν from μ is called the **transition probability** $W(\mu \to \nu)$. For a Markov process, it must satisfy two conditions
  - $W(\mu \to \nu)$ should not vary over time.
  - $W(\mu \to \nu)$ depend only upon $|\mu\rangle$ and $|\nu\rangle$.
- **Markov chain:** By the markov process, we can generate a series of states called markov chain,

$$|\mu\rangle_0 \to |\mu\rangle_1 \to \ldots \to |\mu\rangle_M \ldots$$

- **Ergodicity:** It should be possible for us to reach any state starting from any state if we run the chain long enough time.

Markov process

- Suppose we start with a state $|\mu\rangle$. Next we generate a state $|\nu\rangle$ randomly. Probability of going to ν from μ is called the **transition probability** $W(\mu \to \nu)$. For a Markov process, it must satisfy two conditions
  - $W(\mu \to \nu)$ should not vary over time.
  - $W(\mu \to \nu)$ depend only upon $|\mu\rangle$ and $|\nu\rangle$.
- **Markov chain:** By the markov process, we can generate a series of states called markov chain,

$$|\mu\rangle_0 \to |\mu\rangle_1 \to \ldots \to |\mu\rangle_M \ldots$$

- **Ergodicity:** It should be possible for us to reach any state starting from any state if we run the chain long enough time.
- **Detailed balance**: the markov process will generate states with a stationary probability distribution p_μ is the following condition is satisfied,

$$p_\mu W(\mu \to \nu) = p_\nu W(\nu \to \mu)$$

Markov process

- The detailed balance condition gives,

$$\frac{W(\mu \to \nu)}{W(\nu \to \mu)} = \frac{p_\nu}{p_\mu} = e^{-\beta(E_\nu - E_\mu)}$$

Markov process

- The detailed balance condition gives,

$$\frac{W(\mu \to \nu)}{W(\nu \to \mu)} = \frac{p_\nu}{p_\mu} = e^{-\beta(E_\nu - E_\mu)}$$

- **Metropolis algorithm**: Choose the transition probability to be

$$W(\mu \to \nu) = min\left\{1, e^{-\beta(E_\nu - E_\mu)}\right\}$$

Markov process

- item

Monte Carlo simulation

- item

Thank You.