Monte Carlo Simulation

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1 Metropolis Hastings Algorithm

Suppose ρ be a probability distribution over a space X and suppose $r : X \times X \to \mathbb{R}$ is the relative probability function

$$r(x, y) = \frac{\rho(x)}{\rho(y)}$$

In practice, it is often much easier to compute r than ρ. The Metropolis Hastings algorithm is a Markov chain algorithm that generates samples from X with distribution ρ, given r.

A Markov chain is a sequence of random numbers that are generated iteratively by sampling from a transition probability distribution T. Concretely, if x_k is the kth element in the sequence, x_{k+1} is chosen with probability $T(x_{k+1}, x_k)$. Our goal is to find T such that the sequence of random numbers eventually follow ρ. A sufficient condition for this is known as the principle of detailed balance

$$T(y, x)\rho(x) = T(x, y)\rho(y), \quad \forall x, y \in X$$

intuitively, this means that there is equal probability to transition between any two points in the samples of the distribution ρ.

The algorithm splits the transition into two step: proposal and acceptance. In the proposal step, a point x_p is proposed to be the $(k + 1)$th element by sampling from the distribution $g(x_p, x_k)$, this is usually a function that has high probability for x_p 'close' to x_k. In the acceptance step, we accept the proposed point x_p with probability $A(x_p, x)$. Substituting back to the detaile balance equation, we get

$$\begin{aligned} A(y, x)g(y, x)\rho(x) &= A(x, y)g(x, y)\rho(y) \\ \implies \frac{A(y, x)}{A(x, y)} &= r(y, x)\frac{g(x, y)}{g(y, x)} \end{aligned}$$

We have reduced the problem of finding T to finding A. In this algorithm, we choose A to be defined as

$$A(y, x) = \min\left(1, r(y, x)\frac{g(x, y)}{g(y, x)}\right)$$

2 Ising Model

The Ising model is a d dimensional lattice of length $L - 1$ in each dimension with a spin at each coordinate that may take values ± 1. The state of the system is completely determined by the values of the spins, for a microstate S, $S_{[i]}$ denotes the value of the spin at coordinate $[i]$. The Hamiltonian of the microstate S can be written as

$$H(S) = -\sum_{[i],[j]} S_{[i]}S_{[j]}$$

where the summation is over nearest neighbors $[i], [j]$.

The partition function and thus the pdf for this model is difficult to compute, however r given by

$$r(S_1, S_2) = \exp\left(-\frac{H(S_1) - H(S_2)}{k_B T}\right)$$

is easy to compute especially when S_1 is 'close' to S_2. Therefore, we simulate with Metropolis Hastings with g given by:

$$g(S_p, S) = \begin{cases} \frac{1}{L^d} & S_p \text{ differs from } S \text{ at exactly 1 point} \\ 0 & \text{otherwise} \end{cases}$$

Clearly this g is symmetric ($g(x, y) = g(y, x)$), therefore A simplifies to

$$A(y, x) = \min(1, r(y, x))$$