Monte Carlo Simulation and Its Application

Kshetrimayum Newton Singh

Abstract

Monte Carlo methods (or Monte Carlo experiments) are a class of computational algorithms that rely on repeated random sampling to compute their results. Monte Carlo methods are often used in computer simulations of physical and mathematical systems. These methods are most suited to calculation by a computer and tend to be used when it is infeasible to compute an exact result with a deterministic algorithm. This method is also used to complement theoretical derivations.

In this project we are trying to use this method for finding value of π, numerical integration and 2-d Ising model.

1 Finding the value of π

For finding the value of π, one way is to find the area of a circle and from the equation given below we can find it.

$$\text{Area, } \Delta = \pi R^2 \tag{1}$$

provided R is the radius of the circle. First we consider a square and inside it there is also an in-circle whose radius is unity for simplicity. Now we are going to consider only the first quadrant of the square i.e. area of the square in first quadrant is unity. Now we are generating random numbers between 0 and 1, and count the points which is inside the square and the quarter of the circle.

$$\text{Area of the square, } R^2 \propto N_{square} \tag{2}$$

where N_{square} is # of points hit inside the square.

Area of the circle in the first quadrant,

$$\frac{1}{4}\pi R^2 \propto N_{circle} \tag{3}$$

where N_{circle} is the # of points hit inside the area of the circle in 1st quadrant.

Dividing we can find the value of π as

$$\pi = \frac{4 \times N_{circle}}{N_{square}} \tag{4}$$

Since we can count the number of points hit inside the square as well as inside the quarter of the circle, we can find the value of π. The more points is generated greater is the accuracy.

2 2-D Ising Model

One of the most important uses of the Monte Carlo Simulation in statistical physics is its application in Ising model. Ising model is a statistical model, which was originally used to study the behavior of magnetic particles in a magnetic field. The model consists of a collection of spins on lattice sites. Each spin takes only the value of $+1$ (up) or -1 (down). The model has also been used to study alloys, where instead of representing the lattice site as spins it represents what type of atom is in that site. Say if a site is of the A-type atom, than we can assign 1 or otherwise 0, also same condition for B-type atom.

We can define a Hamiltonian for a system that is dependent on the arrangement of spins on a lattice and from that deduce properties such as magnetization and susceptibility. Suppose that the Hamiltonian is

$$H = -J \sum_{<ij>} S_i S_j - \mu B \sum_i S_i \tag{5}$$

provided J and B are exchanged interaction between nearest spins and magnetic field strength respectively and μ is the magnetic moment possess by the lattice sites. The variable S_i denotes a spin of i^{th} site and can take values either $+1$ or -1.

For the case of $B = 0$, even if the external magnetic field is not applied to the system, there is still a spontaneous magnetization after lowering the temperature of the system to a certain value called *critical temperature* (T_c) where the second-order phase transition happens from paramagnet to ferromagnet. Below the critical temperature, therefore, the spins of all atoms are oriented in the same direction. As a result the material develops non-zero magnetization. This type of transition can be modeled using Monte Carlo.

To analyze this spontaneous magnetization where $B = 0$, we are going to use "the spin-flipping method". The Hamiltonian in ths case is given by

$$H = -J \sum_{<ij>} S_i S_j \tag{6}$$

For a positive J, the above equation takes the minimum value if all the spins are aligned. In statistical mechanics, the all-down configuration is most probable, but other configurations also exist with a probability proportional to the Boltzmann factor e^{-H/k_BT}. For an $L \times L$ two-dimensional lattice, each spin index consists of a pair of integers, $i = (\alpha, \nu), (0 \leq \alpha, \nu \leq L-1)$. The nearest four neighbors of grid point (α, ν) are, $(\alpha \pm 1, \nu)$ and $(\alpha, \nu \pm 1)$. Used to simulate bulk systems without surface effects. It allows a wrap-around condition. For an $L \times L$ two-dimensional lattice, grid points $(L-1, \nu)$ and $(0, \nu)$ are east-west neighbors and $(\alpha, L-1)$ and $(\alpha, 0)$ are north-south neighbors.

The simulation consists of a series of single-spin updates. One grid point, (α, ν), is flipped and the corresponding change in energy is calculated. The spin flip is accepted or rejected according to the Metropolis algorithm. In each MC step, one grid point on the lattice is randomly selected. Take the Hamiltonian as

$$H = -J \sum_{<ij>} S_i S_j \tag{7}$$

Let us consider a 2-dimensional lattice model whose state on each lattice site can only be spin-up ($S = +1$) or spin-down ($S = -1$). Based on this setup, we can now describe the Ising model which possesses the energy given by the above equation. With this Hamiltonian (energy), we can carry out a classical Monte Carlo simulation using Metropolis algorithm as follows.

1. Initially align all spins on the 2D model lattice to up, i.e. $S = +1$.
2. Randomly choose a lattice site i and determine its initial energy E_i and attempt to flip the spin, i.e. from up to down or vice versa and calculate E_j.
3. If flip involves energy downhill i.e. $E_j \leq E_i$, accept the move.
4. Otherwise if $E_j > E_i$, generate a uniformly distributed random numbers $q \in [0, 1]$, accept the move if $q < e^{-\beta(E_j - E_i)}$.
5. If rejected, do not flip the spin and propose another flip at a new random lattice site.
6. If accepted, flip the spin and propose another flip at a new random lattice site.
7. Repeat this again and again, until the "system" is thermalized.
8. After the thermalization stage, one can start making measurements.

To find the magnetization, just sum up all the spins after flipping the spins in the above steps,

$$M = \mu \sum_{i}^{N} S_i \tag{8}$$

or magnetization per spin is

$$m = \mu \sum_{i}^{N} \frac{S_i}{N} \tag{9}$$

provided N is the total number of spin. Also by varying the temperature of the system, we can find the phase transition curve which is plotted between magnetization and temperature.

For the case of non-zero magnetic field i.e. $B \neq 0$, then we can find a relation between magnetization per spin and the applied external magnetic field. In 1-D Ising model the relation between them is given as

$$m = \mu \tanh(\beta\mu B + \beta J m) \tag{10}$$

where $\beta = 1/\kappa T$. Hence the magnetization depends the direction of magnetic field whether the magnetization is up or down.

3 Numerical Integration

The Monte Carlo method can be used to numerically approximate the value of an integral. For a function of one variable the steps are:

(i) pick n randomly distributed points $x_1, x_2, ..., x_n$ in the interval $[a, b]$.

(ii) determine the average value of the function

$$< f >= \frac{1}{n} \sum_{i=1}^{n} f(x_i) \tag{11}$$

(iii) compute the approximation to the integral

$$\int_a^b f(x)dx \approx (b-a) < f > \tag{12}$$

(iv) an estimate for the error is

$$\sigma \approx (b-a)\sqrt{\frac{< f^2 > - < f >^2}{n}} \tag{13}$$

Every time a Monte Carlo simulation is made using the same sample size it will come up with a slightly different value. Larger values n of will produce more accurate approximations. The values converge very slowly $O(n^{-1/2})$. This property is a consequence of the Central Limit Theorem.