Chapter 8

Monte-Carlo Simulation

For scattering, each collision occurs randomly. For integral in high dimension, the number of grid points becomes very large even if each component has small number of grid points. A system with very high degree of freedom is able to be treated only by statistical method. In statistical physics partition function for a system of N particles is

$$Q = \int d^3r_1 d^3r_2 \cdots d^3r_N \exp\left[-\beta\left(\sum_i \frac{p_i^2}{2m_i} + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)\right)\right]. \quad (8.1)$$

Brownian motion of pollen may be described by random walk.

8.1 Monte-Carlo Method

Numerical integral in 1-dimension is approximated as

$$I = \int_0^1 f(x)dx \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i) = I_N \quad (8.2)$$

for equally spaced grid with size $h = 1/N$. In a Monte-Carlo method N points are chosen randomly between $0 \le x \le 1$. The error σ_I of Monte-Carlo integral I_N is, from Eq.(10.6),

$$\sigma_I^2 = |I - I_N|^2 = \frac{\sigma_f^2}{N} = \frac{1}{N-1}\left[\frac{1}{N}\sum_{i=1}^{N} f_i^2 - \left(\frac{1}{N}\sum_{i=1}^{N} f_i\right)^2\right]. \quad (8.3)$$

The standard deviation σ_I of I_N is smaller for larger N with $N^{-1/2}$. For a large N, the randomly chosen x_i are distributed uniformly between $0 \le x_i \le 1$. The integral I_N for a slowly varying smooth function $f(x)$ converges to the exact integral I fast with smaller N than for a fast varying function.

For integral in d-dimensional space, each point is randomly picked by a set of d random values. As an example

$$\pi = 4\int_0^1 dx \int_0^1 dy\theta(1-x^2-y^2) \approx 4\frac{1}{N}\sum_{i=1}^{N}\theta(1-x_i^2-y_i^2) \quad (8.4)$$

where $\theta(r)$ is a step function which is 1 for $r > 0$ and is 0 for $r < 0$. The random points (x_i, y_i) are picked by a pair of random numbers x_i and y_i between 0 and 1. This integral can also be done by throwing coins. Draw a square of side 1 m and draw a quarter circle of radius 1 m centered at one corner of the square. Then throw coins blindly to the square. The ratio of the total number of coins landed in the quarter circle to the number of coins landed in the square is the value of the integral.

If a function $f(x)$ can be factorized to a slowly varying function and a well known positive weighting function $w(x)$ with

$$\int_0^1 w(x)dx = 1 \quad (8.5)$$

the integral can be rewritten as

$$I = \int_0^1 dxf(x) = \int_0^1 dxw(x)\frac{f(x)}{w(x)} = \int_0^1 dy\frac{f(x(y))}{w(x(y))} \quad (8.6)$$

where

$$y(x) = \int_0^x dxw(x) \quad (8.7)$$

which is a solution of

$$\frac{dy(x)}{dx} = w(x) \quad (8.8)$$

with the boundary condition of $y(0) = 0$ and $y(1) = 1$. Then

$$I \approx \frac{1}{N}\sum_{i=1}^{N}\frac{f(x(y_i))}{w(x(y_i))} \quad (8.9)$$

with random number y_i distributed uniformly in $0 \leq y_i \leq 1$.

For a uniformly distributed y_i, the random number $x_i = x(y_i)$ are distributed in the form of function $w(x)$ which is a non-uniform distribution. If the function $w(x)$ has an analytical inverse function $w^{-1}(y)$ then the distribution of the random number $x_i = w^{-1}(y_i)$ is $w(x)$. If $w(x)$ has no analytical inverse then we can use numerical method to find non-uniformly distributed x_i from uniformly distributed y_i. Choose uniformly distributed M values by $y_i = i/M$ in order with $i = 1, 2, \cdots, M$. Then use $\frac{dy}{dx} = w(x)$ to find $x_i(y_i)$ numerically as

$$x_{i+1} = x_i + \frac{y_{i+1} - y_i}{w(x_i)} = x_i + \frac{1}{Mw(x_i)}. \tag{8.10}$$

For random number y which is different from one of the y_i, the corresponding random number x can be found using interpolation with $y_i < y < y_{i+1}$.

8.2 Metropolis Algorithm

Random walk in an empty street requires only one random number for each step. However in a crowded street of metropolis, the realization of next step depends on the occupancy by other person at the next step. The state of scattered particle in a collision of projectile from a target depends on the differential scattering cross section between projectile and target.

For a random walk in a street with a probability density $w(x)$ each step depends on $w(x)$. To move from position x_n to next step x_{n+1} pick x_t by a random number. If

$$r = \frac{w(x_t)}{w(x_n)} \tag{8.11}$$

is larger than 1 then x_t is the next step $x_{n+1} = x_t$ since the probability density at x_t is larger than the probability density at x_n. However, in metropolis Monte-Carlo algorithm, the position x_t is allowed as the next step x_{n+1} if r is larger than a new random number $\eta < 1$ even if $r < 1$. If $r < \eta$ then x_t is not allowed as next step and thus $x_{n+1} = x_n$. In overall randomly chosen new position x_t becomes the next step, i.e., $x_{n+1} = x_t$ if $r > \eta$ and $x_{n+1} = x_n$ without moving to a new position if $r < \eta$ where η is another random number in $0 \leq \eta \leq 1$.