Lecture 10
(Lecture 6 continued)

THE MONTE CARLO METHOD

One-dimensional integral

Consider the integral (normalized):

$$I = \frac{\int_a^b f(x)\, e^{-S(x)}\, dx}{\int_a^b e^{-S(x)}\, dx} = \langle f(x) \rangle$$

Path integral has this form

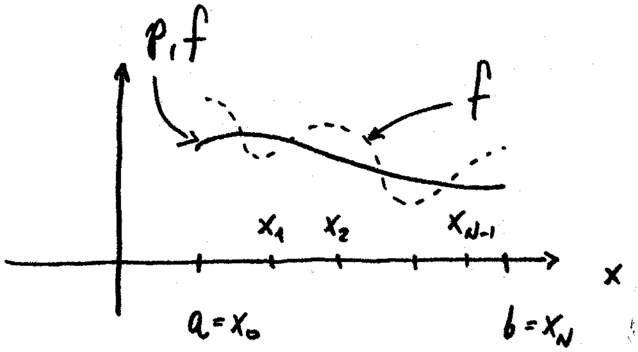
$$Z = \int_a^b e^{-S(x)}\, dx \quad \text{normalization factor}$$

$S(x)$ is some arbitrary real function

$$p(x) = \frac{e^{-S(x)}}{Z}$$ can be considered as normalized probability density

$$I = \langle f \rangle = \int_a^b f(x)\, p(x)\, dx$$

We will use probability theory to evaluate integral



$$\Delta x = \frac{b-a}{N} \qquad N \text{ bins}$$

$$p_i = p\left(\frac{x_{i-1} + x_i}{2}\right) \Delta x$$

$$f_i = f\left(\frac{x_{i-1} + x_i}{2}\right)$$

$$R = \sum_{i=1}^{N} f_i \, p_i \qquad \text{Riemann sum}$$

$$\lim_{N \to \infty} R(N) = \int_a^b f(x)\, p(x)\, dx = I$$

- We will evaluate R with a probabilistic process
- random walk (jump) from cell to cell
- Fixed size (Δx) regular cells are introduced for pedagogical purpose only. At the end of the process they can be eliminated

We start the walker in one of the N cells in (a,b) interval on x-axis

When walker is in cell i, we move it to a new cell j with following rules (importance sampling, Metropolis method):

(1) Select new cell j with equal probability $\frac{1}{N}$

(2) If $e^{-S(x_j)} > e^{-S(x_i)}$, move the walker to cell j

(3) If $e^{-S(x_j)} < e^{-S(x_i)}$, move the walker to cell j

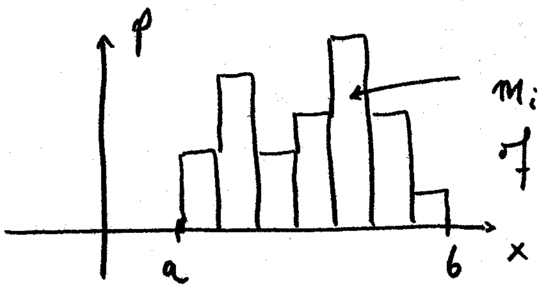
only with probability

$$p = \frac{e^{-S(x_j)}}{e^{-S(x_i)}},$$

otherwise select new cell and start the process again

(4) If walker moved to cell j, go to the beginning of the process and select a new cell again

If walker continues to visit the cells and we make a histogram of how many times a cell was visited after M steps, we should find



m_i: column height of histogram

$$m_i = p_i M$$

becomes exact in $M \to \infty$ limit

$$\overline{f} = \sum_i f_i \frac{m_i}{M} = \frac{1}{M} \sum_i f_i m_i$$

approximates R if M is large enough

for finite M $\overline{f}$ estimates $\langle f \rangle$ with a statistical error (not systematic!)

Error is calculable from variance

$$\sigma^2 = \langle (\overline{f} - f)^2 \rangle \quad \text{constant}$$

$$\pm \frac{\sigma}{\sqrt{M}} \quad \text{error}$$

$$\lim_{M \to \infty} \overline{f} = R$$

$$\frac{1}{M} \sum_i f_i m_i \longrightarrow \sum_i f_i p_i = R$$

Why does it work ?

Consider K independent walkers executing L steps each. The histogram distribution in cells should be the same as the distribution of single walker after $M = KL$ steps

$$L \cdot \underbrace{\frac{k_i}{K}}_{\substack{\text{snapshot} \\ \text{histogram at fixed time}}} = \frac{m_i}{M}$$

$\uparrow$ time integrated histogram of single walker

If $KL = M$, we can think about single walker over long time, or an ensemble K evolving in time

- ✓ L steps of ensemble is equivalent to $M = KL$ steps of single walker
- ✓ If we can prove that $\frac{k_i}{K} = p_i$ for large K, then the single walker will realize the desired distribution
- ✓ Detailed balance guarantees the correct distribution of K ensemble after large enough number of steps, single walker can be used then instead

Steps before equilibrium have to be discarded

$$p_i \, \Pi(i \to j) = p_j \, \Pi(j \to i)$$

DETAILED BALANCE

transition probability

p_i equilibrium probability of state i

Detailed balance is satisfied by Metropolis algorithm:

(a) if $S(x_j) > S(x_i)$ for i, j pair of states

$$\frac{\Pi(i \to j)}{\Pi(j \to i)} = \frac{e^{-S(x_j)} / e^{-S(x_i)}}{1} = \frac{p_j}{p_i} \quad \checkmark$$

(b) if $S(x_j) < S(x_i)$

$$\frac{\Pi(i \to j)}{\Pi(j, i)} = \frac{1}{e^{-S(x_i)} / e^{-S(x_j)}} = \frac{p_j}{p_i} \quad \checkmark$$

If ensemble is in "equilibrium" with the right distribution across the cells, detailed balance will guarantee that the distribution is stationary

If ensemble is not in the right equilibrium distribution, walkers will flee the overpopulated cells in favor of the underpopulated cells

Example $\frac{\rho_i}{\rho_j} = \frac{1}{2}$ for two cells

equilibrium occupancy of cell j is twice of that for cell i

$$\frac{\pi(i \to j)}{\pi(j \to i)} = \frac{\rho_j}{\rho_i} = 2 \qquad \text{detailed balance}$$

for example $\left.\begin{array}{l} k_j = 200 \\ k_i = 100 \end{array}\right\}$ would represent equilibrium

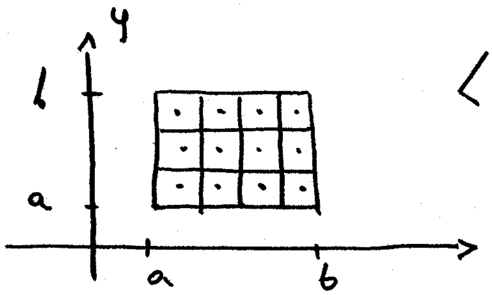
It is two times more likely that particle from cell i moves to cell j, in comparison with opposite move of particle from cell j to cell i. This keeps the right distribution between two cells: same number of particles is exchanged $\rightleftarrows$

$\left.\begin{array}{l} k_j = 400 \\ k_i = 100 \end{array}\right\}$ non-equilibrium situation

Now twice as many particles move from j to i than $i \to j$. System moves towards equilibrium because cell j gets depleted relative to cell i

The discretization of the x-axis can be eliminated completely; a, or b, or both can be infinite

Two-dimensional integral



$$\langle f \rangle = \frac{\int_a^b dx_2 \int_a^b dx_1 \, f(x_1,x_2)\, e^{-S(x_1,x_2)}}{Z}$$

$$Z = \int_a^b dx_2 \int_a^b dx_1 \, e^{-S(x_1,x_2)}$$

Cells are now two-dimensional

$$R = \sum_i f_i \, P_i \qquad P_i = p\left(\frac{x_1^{i-1}+x_1^i}{2}, \frac{x_2^{i-1}+x_2^i}{2}\right)$$

i labels two-dimensional cells $\qquad f_i = f\left(\frac{x_1^{i-1}+x_1^i}{2}, \frac{x_2^{i-1}+x_2^i}{2}\right)$

Same ensemble picture, of random walker

In Metropolis move $i \to j$ from cell to cell, first we select x_1^j coordinate of cell, then we select new x_2^j coordinate in two-step procedure:

Each step is a Metropolis accept-reject procedure

(1) Select new x_1^j with $\frac{1}{N}$ probability

(2) if $S(x_1^j, x_2^i) < S(x_1^i, x_2^i)$ accept

(3) if $S(x_1^j, x_2^i) > S(x_1^i, x_2^i)$

$$\frac{e^{-S(x_1^j, x_2^i)}}{e^{-S(x_1^i, x_2^i)}} \quad \text{acceptance probability}$$

(4) Select now new x_2^j with $\frac{1}{N}$ probability

(5) if $S(x_1^j, x_2^j) < S(x_1^j, x_2^i)$ accept

(6) if $S(x_1^j, x_2^j) > S(x_1^j, x_2^i)$

$$\frac{e^{-S(x_1^j, x_2^j)}}{e^{-S(x_1^j, x_2^i)}} \quad \text{acceptance probability}$$

$i \to j$ move is complete now

Easy to generalize to D dimensions!