Debasis Buxy 2202000914 (1)

Q1.

a) The ~~[illegible]~~ Metropolis Monte Carlo method uses the Metropolis algorithm to generate a random walk of random variables ~~that~~ ~~a~~ according to a distribution function $p(x)$. The random variables ~~[illegible]~~ over a particular interval are then used to estimate the mean value of a ~~[illegible]~~ function, which in turn approximates the value of a definite integral.

To generate a random sequence according to $p(x)$, an arbitrary initial value is first chosen. Then ~~[illegible]~~ each ~~[illegible]~~ step, is governed by a transition probability $T$ ~~[illegible]~~ which follows the principle of ~~the~~ detailed balance (i):

$$p(x_n)\, T(x_n \to x_{n+1}) = p(x_{n+1})\, T(x_{n+1} \to x_n)$$

(ii) The choice of $T$ is defined by:

$$T(x_n \to x_{n+1}) = \min\left(1, \frac{p(x_{n+1})}{p(x_n)}\right)$$

which is consistent with the principle of detailed balance.

(iii) Steps of implementing the method.

a) Generation of random numbers following $p(x)$.

1) Choose initial position $x_0$ (arbitrary).

2) Choose $\delta$ (arbitrary)

3) Generate a random number $\delta_i$ in the interval $[-\delta, \delta]$

4) Calculate trial position $x_{trial} = x_0 + \delta_i$

5) Calculate transition probability

$$w = \frac{p(x_{trial})}{p(x_0)}$$

6) if $w \geq 1$, accept $x_{trial}$ as a valid position
$$x_1 = x_{trial}.$$
7) if $w < 1$, generate a random number $r$
8) if $r \leq w$, $x_1 = x_{trial}$
9) if $r > w$, reject $x_{trial}$ and
$$x_1 = x_0$$
10) Repeat steps 3 to 9 to get successive positions.

This generates $n$ random numbers following $P(x)$.

b) Calculation of definite integral.

1) for every $x_i$ generated, calculate $f(x_i)$
2) Sum $f(x_i)$
3) Calculate mean $\langle f \rangle = \sum_i \frac{f(x_i)}{n}$
4) Calculate definite integral:
$$I = (b-a)\langle f \rangle$$

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b) ~~let $f(x) = 1$~~

$\therefore \cancel{\int f\, dx = \int_{x_0}^{x_7} f(x)\, dx}$

let $f(x) = 2\pi x$ , $x \in [0,1]$

$x_0 = 1$, $x_1 = 0.02$, $x_2 = 0.58$, $x_3 = 0.22$,
$x_4 = 0.12$, $x_5 = 0.54$, $x_6 = 0.81$, $x_7 = 0.07$

$x_i$s are the random numbers $\in$ in $[0,1]$ (given)

$\therefore \langle f \rangle = \frac{1}{n}\sum_{i=0}^{7} f(x_i)$ (Calculate mean of $f(x_i)$)

$= \frac{1}{8}\, 2\pi\, (1 + 0.02 + 0.58 + 0.22 + 0.12 + 0.34 + 0.61 + 0.07)$

$= 2.64$

$\therefore \int_0^1 2\pi x\, dx \simeq 2.64 \quad (b=1, a=0)$

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c)

$$\rho(x) = \begin{cases} c & \text{if } x \in [a,b] \\ 0 & \text{otherwise} \end{cases}, \quad c>0$$

$$\text{Mean} = \frac{\int_a^b x\rho(x)\, dx}{\int_a^b \rho(x)}$$

$$= \frac{\int_a^b c\, x\, dx}{\int_a^b c\, dx} = \frac{\frac{c(b^2-a^2)}{2}}{c(b-a)}$$

$$= \frac{b+a}{2}$$

Variance.

$$= \langle x^2 \rangle - \langle x^2 \rangle$$

$$= \frac{\int_a^b x^2 \rho(x)\, dx}{\int_a^b \rho(x)\, dx} - \left(\frac{\int_a^b x\rho(x)\, dx}{\int_a^b \rho(x)\, dx}\right)^2$$

$$= \frac{\frac{c}{3}(b^3-a^3)}{c(b-a)} - \left(\frac{b+a}{2}\right)^2$$

$$= \frac{b^2+ab+a^2}{3} - \frac{b^2+2ab+a^2}{4}$$

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$$= \cancel{b^2 + ab}$$

$$= \frac{b^2+ab+a^2}{3} - \frac{b^2+2ab+a^2}{4}$$

$$= \frac{4b^2+4ab+4a^2-3b^2-6ab-3a^2}{12}$$

$$= \frac{b^2-2ab+a^2}{12}$$

$$= \frac{(b-a)^2}{12}$$