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Department of Physics
Departmental Semester-End Examinations: December, 2021
M. Sc. (Physics) [Academic Flexibility]

Methods of Computational Physics, Section - I
Date: 10 December, 2021 Time: 3:00 p.m. – 04:00 p.m.
Maximum Marks: 20

Answer any ONE of the questions Q1 and Q2. Usual notation is used. Note: DO NOT use FORTRAN code in your answers.

A uniform random number sequence over the interval $[0, 1]$ is provided at the end. Where required use numbers from the this sequence in the same order.

All calculations are expected to be done by hand. No program is required. In numerical calculations show all numbers rounded off to two decimal figures.

All explanations should be brief and to the point.

Answers should be uploaded as a single pdf file.

Q1 **(a)** Describe the Metropolis Monte Carlo method for estimating definite integrals. Following must be discussed in the description: **(i)** condition of detailed balance, **(ii)** a choice of transition probability that is consistent with the detailed balance, **(iii)** main steps in the algorithm that implements this method.

(b) Estimate the area of a unit circle using Monte Carlo sample mean method (*not* Metropolis!). Use the sample size of $n = 8$. Start with initial value $x_0 = 1$. All the steps in the calculation should be explicitly shown and briefly explained.

(c) Derive the mean and variance of the uniform probability density disbution

$$\rho(x) = \begin{cases} c, & \text{if } a \leq x \leq b; \\ 0 & \text{otherwise} \end{cases}$$

where $c > 0, a, b$ are constants.

(07+08+05)

Q2 **(a)** Use Metropolis Monte Carlo method to generate random numbers which are distributed according to the probability density

$$\rho(x) = \begin{cases} ax(x-1), & \text{if } 0 \leq x \leq 1; \\ 0 & \text{otherwise} \end{cases}$$

where $a > 0$ is a constant. Take the initial value $x_0 = 0.5$, step size $\Delta x \in [-\delta, \delta]$ with $\delta = 0.3$. Calculate $n = 4$ first random numbers. All the steps in the calculations should be explicitly shown and briefly explained (specifically mention acceptance and rejection).

(b) A decrete random variable X takes two values 1 and -1 with probabilities $1/3$ and $2/3$ respectively. Estimate the expectation value $\langle X \rangle$ using Metropolis Monte Carlo method with a sample size of $n = 10$. All the steps in the calculation should be explicitly shown and briefly explained (specifically mention acceptance and rejection).

(10+10)

Random numbers: 0.02, 0.58, 0.22, 0.12, 0.54, 0.81, 0.07, 0.31, 0.94, 0.65, 0.11, 0.48, 0.17, 0.59, 0.67, 0.19, 0.25, 0.44, 0.76, 0.32, 0.46,0.07, 0.95, 0.01,0.57.