13 February 2020

Note : Most of the questions involve transforming a uniform random number(URN) into a random number obeying a different probability distribution. Be clear with transforming a URN into random number from the distribution of interest.

Question 1: Evaluating Integrals using Monte Carlo : Importance Sampling

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a) Evaluate the following integral analytically (pen and paper):

$$I_{real} = \int_0^{\frac{\pi}{2}} sin(x)dx$$

b) Using Random numbers generated from uniform probability distribution function $p(x) = 1$, evaluate the above integral using Monte Carlo method discussed in the class ($I_{uniform}$).
c) Repeat your integral calculation ($I_{importance}$) using random numbers generated from the probability distribution function $p(x) = \frac{8x}{\pi^2}$.

d) Report the data generated in a tabular form with the following columns

1. Trial no.
2. $I_{uniform}$
3. error % observed with $I_{uniform}$
4. $I_{importance}$
5. error % observed with $I_{importance}$

e) Generate a plot using the above data using trial number (x-axis) and observed error with uniform sampling and importance sampling (y-axis).

f) Comment on the observations in (d) and (e). you might also be interested in looking at a plot of $\sin(x)$, $p(x) = 1$ and $p(x) = \frac{8x}{\pi^2}$

Question 2: Evaluating Integrals using Monte Carlo : Importance Sampling

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a) Evaluate the following integral analytically (pen and paper):

$$I_{real} = \int_0^1 \exp(-x)dx$$

b) Using Random numbers generated from uniform probability distribution function $p(x) = 1$, evaluate the above integral using Monte-carlo method discussed in the class ($I_{uniform}$).
c) Repeat your integral calculation ($I_{importance1}$) using random numbers generated from the probability distribution function $p(x) = 1 - x$.

d) Think of a pdf function that can sample better than the ones used above to estimate the integral ($I_{importance2}$)

d) Report the data generated in a tabular form with the following columns

1. Trial no.
2. $I_{uniform}$
3. error % observed with $I_{uniform}$
4. $I_{importance1}$
5. error % observed with $I_{importance1}$
6. $I_{importance2}$
7. error % observed with $I_{importance2}$

e) Generate a plot using the above data using trial number (x-axis) and observed error with uniform sampling, importance sampling1 and importance sampling2 (y-axis).

Question 3: Generating velocities in an MD simulation: Sampling from Maxwell-Boltzmann Distribution

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As you will see in the coming classes, any Molecular Dynamics simulation requires initial conditions which comprises of positions and velocities for each and every particle of the system. The positions are either generated from experimental data or modelled using a protocol specific to each type of molecule/system. The velocities are then generated by sampling the velocities from Maxwell-Boltzmann distribution corresponding to the temperature of interest.

$$p(v) = \left(\frac{m}{2\pi kT}\right)^{\frac{1}{2}} e^{-mv^2/2kT}$$

we can see that this is indeed a gaussian probability distribution function.

$$p(x) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{2}} e^{-x^2/2\sigma^2}$$

Use your URN to generate velocities from this distribution. Generate atleast 1000 such numbers and show that that they indeed obey a gaussian distribution.