P342: Computational Lab
Project/ Assignment 8

Soumik Bhattacharyya
Roll No.-1811155

Discussion on the problems

1   Random Walk Problem

In this problem, graphs of random walk in 2D has been plotted and analysed. For that, a random θ has been generated and X and Y axes has been associated with respectively the cosine and sine of the angle. As the step size is constant and equal to 1, there is no need to multiply step size with $\cos\theta$ or $\sin\theta$. Hundred different random walk has been generated using 5 different set of steps (N= 250, 500, 800, 1200 and 1500). First five of them has been plotted for each N; radial distance R, R_{rms} and average displacement in both axes has been found out and R_{rms} vs $\sqrt{N}$ graph has been plotted.

The R_{rms} vs $\sqrt{N}$ has been found to be a straight line (verified for reasonably high values of set of steps). It matches well with the analytical result, because according to the diffusion equation square root of time is proportional to the rms displacement of the molecule.

2   Monte Carlo Problem

In this problem, the volume of an ellipsoid has been found out with Monte Carlo method with the values of a, b and c given. For that, 96 trials have been taken, with step number N= 100, 600, 1100, ...49600.

The analytical solution is 12.57 $unit^3$. In a plot, the numerical value in Monte Carlo for each N has been plotted and compared with analytical solution. With increasing N, it converges with the analytical solution. Subsequently, error is reduced for increasing N. Also, it has been validated using a plot.

Later, a 3-D plot of the ellipsoid has been projected using numerical value by Monte Carlo with a large value N (25000).