Modeling and Simulation, CS302

Lab-6

Due-Date: March 8, 2017

Modeling with randomness. Problems (1) and (2) are required. Q. 3 is not a part of the lab but interested students can get a feel of Markovian vs non-Markovian random walks.

1. **(Radioactive decay)**

   (a) We have in the initial lectures modeled radioactive decay as a deterministic process. But radioactive decay is a nondeterministic process which can be simulated very naturally using the Monte carlo method. Suppose that the probability of any atom decaying over a time interval Δt is given by λ $(0 < \lambda < 1)$. Then the history of a single atom can be simulated by choosing a sequence of random numbers x_k, $k = 1, 2, ...m$ uniformly distributed on $[0, 1]$. The atom survives until the the first value of x_k for which $x_k < \lambda$. Use this approach to simulate an ensemble of atoms remaining after k intervals. Take $\lambda = 0.1$ and $m = 50$ and try values $n = 10, 100, 1000$ and 10000. How does the value of n (ensemble size) affect the smoothness of the resulting curve. Experiment with other values λ, n and m.

   (b) Compare your results with the continuous, deterministic model of radioactive decay. Which model do you think is closer to the way nature actually behaves and why?

2. **(1D Random walk)**

   (a) **(Symmetric random walk**) In this first part we will simulate the symmetric random walk. Let the probability of a random walker going left or right be the same $p = q = 1/2$. The walk starts from the site 0 and proceeds by successive steps of unit length. For direction we adopt the convention that right is positive and left is negative. Write a program to implement the random walk of n steps, using a uniform random number generator to choose the direction of each step. Run your code to calculate the mean and mean square displacement(msd) . What is the size of the ensemble beyond which you observe Einstein's relationship *(Show in a single figure by taking ensemble of different sizes)*. What is the value of Diffusion constant? Make a histogram of of the distribution of $p_n(m)$ obtained from your data, where $p_n(m)$ is the probability of being at the mth site after n steps.

(b) **(asymmetric random walk)** Let us now consider the case of unequal probabilities of going left or right. Such a situation arises quite often when we force the random walker to prefer one of the directions. Think of the motion of an electron inside the metal in the presence of electric field. Let p be the probability of going right and $q = 1 - p$ be the probability of going left. Assuming that the random walker takes unit steps at each step what is the mean distance and mean squared displacement. Compare with the previous case.

(c) **(Walk of varying lengths)** Let us now allow the random walker to take steps of varying lengths. While we can in principle take any distribution for the step length let us assume that the length of the steps are normally distributed with with mean 0 and variance 1. From your simulations comment on the general behavior of the random walker in terms of the mean and msd, and calculate the diffusion constant. If the distribution was not standard normal but rather $N(\mu, \sigma)$ do you observe any difference in the behavior.

3. **(Extra: non-Markovian random walk)** Many physical processes are modeled as non-Markovian or ones in which the random walker has memory of the past. One such analytically tractable model was proposed by Schütz *et al.* (Elephants can always remember, Phys. Rev. E **70**, 045101(R) (2004)), where the next step of the random walker is based on the past history. The steps are of unit length but at each time step the walker looks in to the complete past. The walker for example at time $t + 1$ selects a time t' from the set $\{1, 2...t\}$ with uniform probability. The walker then with probability p decides to take the same step or with probability $1 - p$ the opposite step. At $t = 0$ the walker takes the step $+1$ with probability q and -1 with probability $1 - q$. Analyze the mean squared displacement as a function of p. Do you think that the initial conditions will have an important role to play. Can you identify different regimes in the motion. What if the random walker stayed stationary with a probability r.