CE 530
Molecular Simulation

Assignment #4 Due: 07 March 2017

1. Evaluate the integral of $f(x) = 3x^2$ for $x = 0..1$ using Monte Carlo integration with importance sampling. Use the following weighting functions:
   (a) $p(x) = 1$
   (b) $p(x) = 2x$
   (c) $p(x) = 4x^3$

   Pick a sample size and perform multiple runs of your program (taking care not to begin all runs with the same random-number seed), taking statistics to compute the variance of the values given by the runs. This can also be done in Excel, if you prefer. Compare these results with the variances you would expect from the formula given in class.

   If you wish to use Java (or get some ideas), some Java classes for doing multivariate and Monte Carlo integrations are available at
   http://www.eng.buffalo.edu/%7ekofke/src/montecarlo/

2. Here is a transition probability matrix for a four-state system:

$$\begin{pmatrix} 0.5 & 0.1 & 0.1 & 0.3 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.1 & 0.2 & 0.3 & 0.4 \\ 0.2 & 0.1 & 0.35 & 0.35 \end{pmatrix}$$

   (a) Compute analytically the limiting distribution corresponding to these transition probabilities. Use an algebraic approach, in which you solve the balance equations and normalization, as presented in class.
   (b) Repeat (a), but by computing the appropriate normalized left eigenvector of the matrix.
   (c) Do the transition probabilities and the limiting distribution obey detailed balance?
   (d) Perform a random walk for this set of transition probabilities using the Markov process applet here: http://www.eng.buffalo.edu/~kofke/applets/MarkovApplet1.html. Take a screen shot of the distribution after many steps, and submit that with your assignment.

3. Here is a transition probability matrix for a four-state system:

$$\begin{pmatrix} 0.1 & 0.9 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0 \\ 0 & 0 & 0.3 & 0.7 \\ 0 & 0 & 0.6 & 0.4 \end{pmatrix}$$

   A Markov process that attempts to sample according to these transition probabilities will be flawed. What is wrong?

4. Consider the following probability distribution for a 4-state system:

$$\pi_1 = 0.2 \quad \pi_2 = 0.1 \quad \pi_3 = 0.5 \quad \pi_4 = 0.2$$

(a) Derive a set of transition probabilities according to the Metropolis algorithm that will yield this as the limiting distribution of a corresponding Markov process on the four states.
(b) Use these transition probabilities in the Markov applet to show that they do indeed give the desired limiting distribution. Submit a screenshot of the distribution you get.

5. It is common practice in Monte Carlo simulations to increment a running sum not after each and every elementary Monte Carlo step, but instead to do the increment only after some fixed number of elementary steps have been taken. This might be done, for example, because the calculation involved in getting a value for the current configuration is expensive, and it is not worth doing after every little change in the configuration.

   In effect, this procedure describes a "super-Markov" sequence, in which each subsequent configuration in the sequence is obtained by an intervening series of simpler Markov steps. Show that if the transitions probabilities for the simpler Markov steps obey detailed balance, then the transition probabilities for this super-Markov sequence also obey detailed balance for the same limiting distribution.