Numerical Methods, 2012

Assignment on Monte Carlo Methods

Due on Dec 4, 2012

You have to show working codes

1. Write a code to generate random numbers x that are distributed according to the probability density function $p(x) = \sqrt{1 - x^2}$ in the range $[0, 1]$ using the rejection method.

   Show that your code indeed gives you the desired distribution by doing the frequency test.

   Estimate the value of π using your code. How does your estimate of π change as you increase the number of random points for your estimation? Report π for a few cases.

2. Remember the illustrative example I showed in the class for the transition matrix $\mathbf{P}$ for a 3-state problem

$$\mathbf{P} = \begin{pmatrix} 1/4 & 1/8 & 2/3 \\ 3/4 & 5/8 & 0 \\ 0 & 1/4 & 1/3 \end{pmatrix} \tag{1}$$

   that led to the equilibrium probabilities $p_1^* = 4/15$, $p_2^* = 8/15$ and $p_3^* = 3/15$?

   Consider the inverse problem. Suppose you are given the equilibrium probabilities $p_1^* = 3/15$, $p_2^* = 4/15$ and $p_3^* = 8/15$. Construct the transition matrix $\mathbf{A}$ for a metropolis algorithm for this problem. Now suppose you have a large number of walkers (a few thousand may be a good choice) all in the state 2 at the beginning. In a Metropolis method, at each step try to move each one of them to any of the three states. All the states, to which a move can be attempted, are chosen with equal probability of 1/3. However, the proposed moves are to be accepted with probability given by the matrix $\mathbf{A}$.

   Write a code for this problem, and report how the number of walkers in the three states vary with MC time. You must point out when equilibrium is reached.

3. *I will add one more problem by Monday-Tuesday*