Singapore-MIT Alliance, CME5233 – Particle Methods and Molecular Dynamics

Tutorial 4, Monday 2:30 – 4:00, 27 Nov 2006

1. (a) Let assume that the transition matrix W_i has invariant distribution P for all i, i.e., $P = P\ W_i$, i=1,2,..,N. show that both the weighted sum $W_s = \Sigma_i \lambda_i W_i$ and product $W_p = \Pi_i W_i$ have invariant distribution P, where $\Sigma_i \lambda_i = 1$, $\lambda_i > 0$. How to implement W_s and W_p on computer?
(b) If W_i satisfies detailed balance with respect to P, is W_s and/or W_p satisfy detailed balance?

2. Show that the Metropolis transition probability
$$W(X \to X') = T(X \to X') \min\left(1, P(X')/P(X)\right)$$
satisfies detailed balance as long as matrix $T(\ldots)$ is symmetric.

3. The Metropolis algorithm is a general method to produce arbitrary distribution in any dimensions. In this exercise, we consider applying the Metropolis method to a simple 1D distribution of the form $p(\mathrm{x}) = e^{-x}$ for $x \ge 0$ and $p(\mathrm{x}) = 0$ of $x < 0$.
   a. If the current value of the random variable is x, and new one y is obtained by moving x slightly centered round x, and picked at randomly in a box of $[x - 0.1, x + 0.1]$ with uniform distribution, give a formula that generate y using the known value x and a uniformly distributed random number ξ between 0 and 1.
   b. For the above operation (given x, choose a y), write the conditional probability $T[x \to y]$ that appears in Metropolis algorithm.
   c. Give the formula for the transition matrix $W(x \to y)$ in Metropolis algorithm, applied to the present situation.
   d. Specify a set of pseudo-code that gives the precise steps of the Metropolis algorithm that generate required distribution, $P(x)$, for the random variable x. Pay particular attend to the situation when the new variable y becomes negative.