CHM1465: Foundations of Molecular Simulation

PROBLEM SET 1

Notes:

- This set contains 3 problems.
- This first set is due in one week, October 8, 2008.

1. Suppose a Markov chain has the following transition matrix for a three-state system:

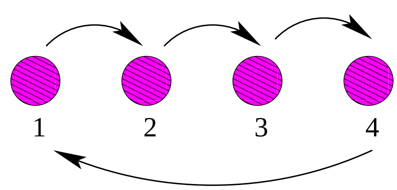
$$\mathsf{K} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

   (a) What are the eigenvalues of K? What independent eigenvectors have eigenvalue $\lambda = 1$?

   (b) If a random walk starts in state 1, what is the probability of finding state 1 after 2 steps? After 3 steps?

   (c) Is the transition matrix regular? Does this random walk have a unique limit distribution?

2. Consider a one-dimensional, time-homogeneous, discrete time, Markovian random walk process in which a walker always moves to its neighbor to the right. Suppose there are 4 sites, and a walker at site number 4 always cycles back to site 1:



   (a) Write down the transition matrix $\mathsf{K}^{(0)}$ for this process and show that the eigenvalues of this matrix are $\lambda_k^{(0)} = e^{-ik\pi/2}$ for $k = 1, \ldots, 4$.

   (b) Show that the right eigenvectors of $\mathsf{K}^{(0)}$ are $\mathsf{e}_k^{(0)} = 1/2\,(e^{i\pi k/2}, e^{i\pi k}, e^{i\pi 3k/2}, e^{i\pi 2k})$ and that the left eigenvectors are the complex conjugates $\mathsf{e}_k^{(0)*}$.

   (c) Now suppose that there is a small but finite probability ϵ that the walker remains on site 1 and probability $1-\epsilon$ to step to site 2. What is the form of $\mathsf{K} = \mathsf{K}^{(0)} + \Delta\mathsf{K}$ now?

   (d) The effect of the perturbation $\Delta\mathsf{K}$ on the eigenvalues can be evaluated using perturbation theory using

$$\lambda_k = \lambda_k^{(0)} + \Delta\lambda_k$$

where $\Delta\lambda_k = \mathsf{e}_k^{(0)*} \cdot \Delta\mathsf{K} \cdot \mathsf{e}_k^{(0)}$, to first order in ϵ. Evaluate the effect to first order in ϵ of the perturbation on the eigenvalues λ_k. Does the perturbed system have a unique limit distribution?

(e) What is the effect of the perturbation on the eigenvector e_4? What is the physical meaning of this eigenvector?

3. Consider a circle of diameter d contained in a square of side length $l \geq d$.

(a) Construct an estimator for π using the fraction of uniformly selected points in the square that fall in the circle and show that the average of this estimator over the true (uniform) distribution is π.

(b) Derive an expression for the standard error in the estimated value of π using this algorithm. How does it depend on N (number of points sampled) and the ratio l/d? For fixed l what is the optimal value d that minimizes the standard error?

(c) Write a schematic (or explicit) computer program to compute the value of π using this method.