Bioinformatics: Practical Application of Simulation and Data Mining: Homework 2

March 1, 2010

Due: Friday, March 19, 2010

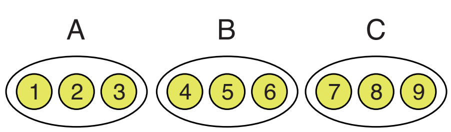
Markov Processes in 9-Microstate Model

The 9-microstate model system described in *J. Chem. Phys.* **131** (2009) 124101 and the corresponding transition matrix are shown in Fig. 1.

(i) Use detailed balance among all microstates to find the steady-state probability distribution, *i.e.* how likely is the system to be in states 1-9 at long times? Detailed balance among microstates 1 and 2 is given by

$$T_{12}P_2 = T_{21}P_1, \tag{1}$$

where T_{ij} is the transition probability from microstate j to i and P_i is the probability to be in microstate i at a given time. There are 8



$$T = \begin{pmatrix} 0.99 & 0.005 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.01 & 0.99 & 0.01 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.005 & 0.986 & 0.004 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.004 & 0.976 & 0.01 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.02 & 0.98 & 0.02 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.01 & 0.976 & 0.004 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.004 & 0.946 & 0.025 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.05 & 0.95 & 0.05 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.025 & 0.95 \end{pmatrix}$$

Figure 1: Representation of the Markov transition matrix for the 9-microstate model. Only off-diagonal values of the matrix are shown in the diagram on the left. The nine microstates are indicated by numbers. The three macrostates, indicated by letters, are formed by lumping groups of three microstates together, as shown.

such equations and an additional constraint on the probabilities

$$\sum_{i=1}^{9} P_i = 1. \tag{2}$$

(ii) (Programming) Assuming that the system is initially in state 2, calculate the microstate probabilities as a function of iteration number n. To do this, calculate

$$P_i(n) = T_{ij}^n P_j, \tag{3}$$

where $P_j = (0, 1, 0, 0, 0, 0, 0, 0, 0)$. Show that the long-time ($n > 2000$) microstate probabilities agree with what you obtained in problem (i).

(iii) Coarse-grain the microstates into macrostates $A = 1, 2, 3$, $B = 4, 5, 6$, and $C = 7, 8, 9$ according to Fig. 1 using the appropriate Boltzmann weights from part (i). Generate a new coarse-grained transition probability matrix. Calculate the steady-state probabilities of the macrostates using a method similar to problem (i). Show that the steady-state macrostate probabilities correspond to the sum of the microstates for each macrostate.

(iv) Coarse-grain your systems into a different set of macrostates from problem (iii), $A' = 1, 2, 3, 4, 5$, $B' = 6, 7$, and $C' = 8, 9$ using the appropriate Boltzmann weights from part (i). Calculate the steady-state probabilities of the macrostates. Does your answer agree with problem (iii)? Why or why not?

(v) Why are eigenvalues of the transition matrix important? (Programming) Calculate

$$P_i(n) = T_{ij}^n P_j, \tag{4}$$

where $P_j = (0, 1, 0, 0, 0, 0, 0, 0, 0)$, but approximate T_{ij}^n using only its largest eigenvalue. Calculate $(P_j(\text{largest eigenvalue}) - P_j(\text{exact}))^2$ as a function of time for $n = 0$ to $n = 2000$.