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Computational Molecular Physics **Winter 2017/18**

Problem set 5 — 30 November 2017

Problem 5.1 *Stochastic matrices*

a) *(Periodic, deterministic Markov chain)*
Assume a four-state Markov chain with the (column-stochastic) transition matrix

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

Draw the graph of the Markov chain. Determine the eigenvalues and eigenvectors of T and plot the spectrum on the complex plane. Verify that there is one largest eigenvalue that is real, positive, and simple, and that this is the only eigenvalue with non-negative eigenvectors. Which symmetry does the spectrum exhibit? (Hint: $T^4 = \mathbb{1}$.) What does this imply for $\lim_{k\to\infty} T^k$? Is the Markov chain ergodic?

b) *(Aperiodic, non-equilibrium Markov chain)*
Now, consider the modified transition matrix

$$T = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1/3 & 0 & 0 & 0 \\ 1/3 & 1 & 0 & 0 \\ 1/3 & 0 & 1 & 0 \end{pmatrix}.$$

Draw the graph of the Markov chain and repeat the analysis from part a). Discuss the changes in the spectrum and how this affects the convergence to the stationary distribution. Why does this distribution not describe an equilibrium situation?

c*) *(Asymptotically periodic Markov chain)*
If the first column of T is replaced by $(0, 1/2, 0, 1/2)$, the Markov chain is asymptotically periodic as $k \to \infty$. Again, draw a graph of the chain, determine the spectrum of T and the stationary distribution. Demonstrate asymptotic periodicity by evaluating powers T^k for large k. What is the period of the Markov chain? Is such a chain ergodic?

Let $p(0)$ be some initial probability distribution and define $p(k) := T^k p(0)$ for $k \in \mathbb{N}$. Give two distributions $p(0)$ such that the sequence $p(k)$ converges and two distributions such that it does not. Specifically, test numerically whether $\|p(k+1) - p(k)\| \to 0$ for $k \to \infty$ or not.

Problem 5.2 *Transition probabilities*

The files *"data1.txt"*, *"data2.txt"*, and *"data3.txt"* each contain sequence of states i.e., $[1, 2, 3]$ sampled by Markov Chain Monte-Carlo.

a) Plot the histograms of each sequence. How do the distributions differ for the three sequences?

b) Determine the transition probabilities between the states for each sequence.

c) Check whether any of the sequences obey detailed balance i.e., $\pi(i)\mathrm{P}(\mathrm{i}\to\mathrm{j}) = \pi(j)\mathrm{P}(\mathrm{j}\to\mathrm{i})$?

Due date: ***7 December, 12 p.m.***