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Computational Molecular Physics **Winter 2017/18**

Problem set 4 **24 November 2017**

Problem 4.1 *Transition matrix*

a) Consider the Markov chain with four states, that has the following transition matrix

$$\mathbf{P} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

b) Draw a diagram representing the states (e.g. as circles) and transitions (as arrows) for this chain.

c) Given the following vectors of probabilities of the four states

$$\mathbf{w}_1 = \begin{pmatrix} 1/6 & 2/6 & 2/6 & 1/6 \end{pmatrix}^\mathsf{T},$$
$$\mathbf{w}_2 = \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \end{pmatrix}^\mathsf{T},$$
$$\mathbf{w}_3 = \begin{pmatrix} 1/2 & 1/4 & 0 & 1/4 \end{pmatrix}^\mathsf{T},$$

check whether any of them represents a stationary distribution.

d) Apply the transition matrix to the distributions $\mathbf{w}_1$, $\mathbf{w}_2$, and $\mathbf{w}_3$ once, twice, n times. That is compute ${\mathbf{w}_i}^\mathsf{T}\mathbf{P}^n$ for $n = 1, 2, \ldots, 7$. What do you observe?

e) Find eigenvalues and corresponding eigenvectors (left and right) of the transition matrix. How can the eigenvalues and eigenvectors be understood in a more physical meaning?

Problem 4.2 *Markov model from a trajectory*

The file *"dtraj.txt"* contains a modified sequence of states, i.e., $[0, 1, 2, 3, 4, 5, 6, 7]$, extracted from the molecular dynamics trajectory of Alanine-Leucine after partitioning the selected torsion angles space.

a) Plot the discrete trajectory and compute the transition matrix for it.

b) Calculate eigenvalues and left eigenvectors of the transition matrix.

c) Plot the first four eigenvectors of the transition matrix. Comment on the stationary distribution, i.e., the 1$^{\text{st}}$ eigenvector, and which state transitions do you observe from the 2$^{\text{nd}}$ and 3$^{\text{rd}}$ eigenvectors?

d*) Split given states into sets/clusters using the sign structure of the 2$^{\text{nd}}$ and 3$^{\text{rd}}$ eigenvectors. Plus make a diagram which shows the most frequent transtions between the found clusters.

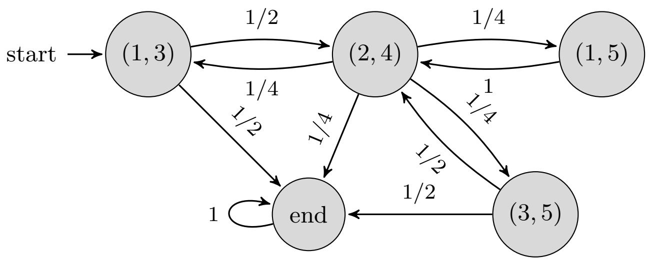
(please turn over)

Problem 4.3 *The cat and the mouse*

Suppose you have five adjacent boxes, with a cat initially in the first box and a mouse in the last. After each fixed time interval, the cat and the mouse jump randomly to one of the adjacent boxes, each independently and with equal probability for all directions. (The first and the fifth box have only one adjacent box.) The "game" ends when the cat and the mouse meet in the same box.

The possible states are denoted by index pairs (i, j), i.e., the cat sits in box i and the mouse in box j. The state space is considerably reduced by noting that $i \leq j$ and that i and j are both either odd or even; the terminal states have $i = j$ and can be merged into a single state. The accessible state space is thus $S = \{(1,3), (1,5), (2,4), (3,5), \text{end}\}$.

a) Justify the following transition graph of the Markov chain and write down the transition matrix $T \in \mathbb{R}^{5\times5}$:



b) Verify that T is a column-stochastic matrix, i.e., $T_{mn} \geq 0$ for all m, n and $\sum_m T_{mn} = 1$ for all n. Determine the eigenvalues λ_i $(i = 1, \ldots, 5)$ and right eigenvectors u_i of T (making use of computer algebra). Plot the spectrum of T in the complex plane and confirm the statements of the Perron–Frobenius theorem. What is the stationary distribution p^{s} of the Markov chain?

c*) Compute matrix powers T^k for $k = 1, 2, \ldots, 50$ and verify that the columns of T^k converge to p^{s}. Let $q_1 = (1, 0, \ldots, 0) \in \mathbb{R}^n$ and plot $E(k) := \|T^k q_1 - p^{\mathrm{s}}\|$. Find the convergence rate γ from the slope of $\log(E(k))$ vs. k as $k \to \infty$. Compare $\mathrm{e}^{-\gamma}$ with the second-largest eigenvalue of T.

Hint: This problem is also an exercise in translating between different conventions used by different communities. Here, T is a column-stochastic matrix since the elements of T are defined as $T_{mn} = \mathrm{P}(m \leftarrow n)$. Then the left and right eigenvectors change their roles. The convention used in the lecture is restored by using the transpose, T^{T}.

Due date: ***30 November, 12 p.m.***