

Problem set 5: Computational Molecular Physics and Methods of Molecular Simulations

Petra Imhof, Antonia Mey, Burkhard Schmidt
Department of Physics // Mathematics and Computer Science
Freie Universität Berlin

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1. Markov Chain classification

(30 points) Classify the following transition matrices, whether they are:

- (a) Irreducible
- (b) Ergodic
- (c) periodic
- (d) reversible

$$T_1 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, T_2 = \begin{pmatrix} 0.2 & 0.8 & 0 \\ 0 & 0.2 & 0.8 \\ 0.8 & 0 & 0.2 \end{pmatrix}, T_3 = \begin{pmatrix} 0.7 & 0.3 & 0 \\ 0 & 0.2 & 0.8 \\ 0 & 0 & 1 \end{pmatrix}$$
$$T_4 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0.1 & 0.8 & 0.1 & 0 \\ 0 & 0 & 0 & 0.9 & 0.1 \\ 0 & 0 & 0 & 0.3 & 0.7 \end{pmatrix}, T_5 = \begin{pmatrix} 0.8 & 0.2 & 0 \\ 0.1 & 0.8 & 0.1 \\ 0 & 0.6 & 0.4 \end{pmatrix}$$

2. Transition matrix estimation

(20 points) Use the trajectory of a three state Markov chain provided on the website and estimate a maximum likelihood transition matrix from the data, with a lagtime $\tau = 1$ (i.e. use every data point) and $\tau = 10$ (i.e. only use every 10th data point). Compute the eigenvalues and eigenvectors for both cases of your estimated transition matrix. What do you notice regarding your eigenvalues and eigenvectors. Give an explanation for your observation.