Blatt 4. Markov Processes 2

1. The exercises marked by $\star$ are challenges to think about, to be discussed when we discuss the solutions.
2. Sage has very powerful linear-algebra packages that can caluclate the coefficients of the characteristic polynomial of the skewed transition matrix, and the derivatives involved in finding cumulants.

Problems

4.1. Kolmogorov's Cycle Criterion

The Kolmogorov's Cycle Criterion states that a Markov model represents an equilibrium state iff all circulations of the observable $\Omega := (i \to j) \mapsto \omega^i_j = \log \frac{w^i_j}{w^j_i}$ vanish,

$$\circ\omega_\alpha = \sum_{i \to j \in \zeta_\alpha} \omega^i_j = 0 \quad \text{for all cycles } \zeta_\alpha$$

We proof this statement in three steps.

a) Show that the criterion can be relaxed: It is sufficient when the values $\circ\omega_\alpha$ vanish for the fundamental cycles that are selected by a set of chords.

b) Define the weights g_i by the recursion $g_1 = 1$ and $g_i = w^j_i\, g_j / w^i_j$ when g_j is known.
Why is this a meaningful definition?
What goes wrong when the Kolmogorov's Cycle Criterion does not hold?

c) Let $G := \sum_{i=1}^{N} g_i$ be the sum of the values g_i over all states $i \in \{1, \dots, N\}$. Show that $p_i = g_i/G$ is a probability distribution that is stationary, and that it obeys detailed balance. How does this complete the proof?

4.2. Three interacting particles on four sites (Part 2)

We consider a system with four binding sites on a ring, as previously discussed in problem 3.5: In this system there is one + particle and two $\circ$ particles. Accordingly, there is a tight state $T = [\circ, +, \circ, \_]$ where + has two neighbors, as well as states $L = [\circ, +, \_, \circ]$ and $R = [\circ, \_, +, \circ]$ where + only has a neighbor to the left or right, respectively. Let T decay to L and R with the same rate d, while the reverse processes happen at a rate u. Moreover, the hopping of + is biased: $L \to R$ occurs with rate r and $R \to L$ with rate l.

a) Write down the skewed transition matrix $\hat{\mathsf{W}}$ for an antisymmetric observable ω.
Remark: The (i, j) component of the transition matrix is the transition rate w^i_j to go from state $i \to j$. The (i, j) component of the skewed transition matrix is $w^i_j\, e^{s\,\omega^i_j}$.

b) Determine the characteristic polynomial of the skewed transition matrix,

$$P(\lambda; s) = a_3\, \lambda^3 + a_2\, \lambda^2 + a_1\, \lambda + a_0$$

where (in principle) a_3, a_2, a_1, and a_0 are functions of s (see, however, (d)).

c) Show that a_2 and a_1 do not depend on s, and that a_0 only depends on $\bar{\omega}\, s$, where $\bar{\omega}$ is the sum $\bar{\omega} = \omega_L^T + \omega_R^L + \omega_T^R$ over the contribution to the observable added up for the transitions around the cycle $T \to L \to R \to T$.

d) Verify that $a_0(s)|_{s=0} = 0$. Why should that be true for every transition matrix?

⋆ e) Consider the implicit equation

$$0 = P(\lambda(s); s)\,.$$

Use $\lambda(s)|_{s=0} = 0$ and the implicit function theorem to show that

$$J = \left.\frac{\mathrm{d}\lambda(s)}{\mathrm{d}s}\right|_{s=0} = \frac{-1}{a_1}\; \left.\frac{\mathrm{d}a_0(s)}{\mathrm{d}s}\right|_{s=0}$$

Do you see why this is true for *every* finite Markov process?

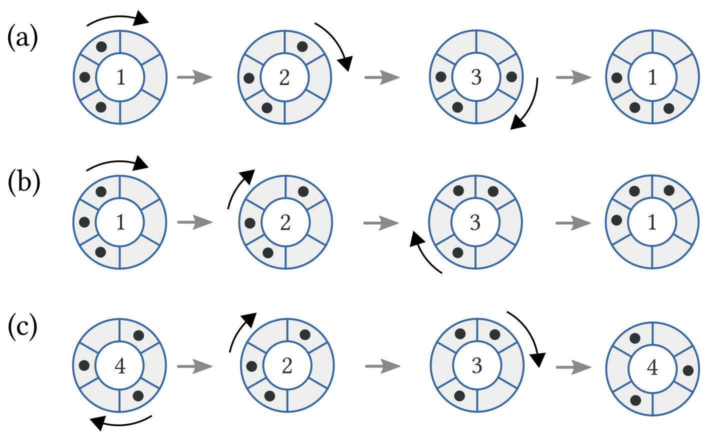
f) Determine the current J for the present example.
How does it differ for different observables ω?

4.3. Simple asymmetric exclusion process for 3 particles on 6 sites

A simple exclusion process is a transport process where particles reside on the sites of a one-dimensional lattice, and they move according to the following rules:

- A lattice stite can be occupied by at most one particle.
- Particles jump to their right neighboring site with a rate r iff the site is empty.
- Particles jump to their left neighboring site with a rate l iff the site is empty.

The process is called an asymmetric simple exclusion process (ASEP) when $r \neq l$, and without loss of generality we will consider then the case $r > l$. Commonly one adopts periodic boundary conditions, arranging the lattice sites on a ring with N sites. In that case one can identify states that only differ by rotation. Here, we consider an ASEP of 3 particles on 6 sites. Up to rotation symmetry the system has four states. The panels (a) and (b) in the figure below show two possibilities to go from state 1 to state 1 by performing three steps in clockwise direction. Panel (c) shows a possibility to go from state 4 to state 4 by performing three steps in clockwise direction.



We will now calculate the particle current and the diffusivity of this transport process.

a) Sketch the graph for this Markov process and mark the transition rates. Marke sure that you appropriately account for cases where there multiple options to perform a transition (for instance the figure shows that there are two possibilities to go from 2 to 3).
Do we have dynamical reversibility? Do we have absorbing states?

b) Write down the transition matrix $\mathbb{W}$ and the skewed transition matrix $\hat{\mathbb{W}}_{\mathcal{D}}$ for the observable $\mathcal{D}$ that counts the number of steps. Calculate the characteristic polynomial $\det(\hat{\mathbb{W}}_{\mathcal{D}} - \lambda\, \mathbb{I}_4)$ and determine the displacement current.

c) Choose the chords $\alpha := 2 \to 3$ and $\beta := 3 \to 4$ to describe the Markov process. Write down the skewed transition matrix $\hat{\mathbb{W}}(\mathbf{q})$ for the chord observables. How does the characteristic polynomial change with respect to part (b)?

d) Determine the cumulants $C(\alpha)$, $C(\beta)$, and $C(\alpha, \alpha)$ for the chord observables.

e) Determine the circulation of $\mathcal{D}$ for the fundamental cycles ζ_α and ζ_β.
Use this result to calculate the displacement current based on $C(\alpha)$ and $C(\beta)$.

f) Up to a factor of two the variance $C(\mathcal{D}, \mathcal{D})$ amounts to the diffusion coefficient of the displacement. Show that *only* $C(\alpha, \alpha)$ is required to calculate this diffusion coefficient based on chord observable. Determine the diffusion coefficient for the displacement.

4.4. Gauge Invariance of Antisymmetric Observables

Let w^i_j be the transition rates between the states $i, j \in \{1, \ldots, N\}$ of a Markov process with N states, and let $\mathbf{g} \in \mathbb{R}^N$ be a vector with components g_i, $i \in \{1, \ldots, N\}$.

a) Show that $\Omega(\mathbf{g}) := (i \to j) \mapsto \omega^i_j(\mathbf{g}) = \log \frac{w^i_j\, g_i}{w^j_i\, g_j}$ is an antisymmetric observable, irrespective of the choice of $\mathbf{g}$.

b) Show that the observables $\Omega(\mathbf{g})$ all have the same cumulants for the distribution of the sum $\omega^i_j(\mathbf{g}) := \sum_{\text{jumps } i \to j} \omega^i_j(\mathbf{g})$ over all jumps performed in the time interval T.
The cumulants are "blind" to the choice of $\mathbf{g}$.

c) Let $\omega(\mathbf{g}_1, T)$, $\ldots$, $\omega(\mathbf{g}_\ell, T)$ be the sums for ℓ different observables $\Omega(\mathbf{g}_1)$, $\ldots$, $\Omega(\mathbf{g}_\ell)$. The mixed cumulant of these observables is obtained as

$$C(\Omega(\mathbf{g}_1), \ldots, \Omega(\mathbf{g}_\ell)) = \frac{1}{T} \frac{\mathrm{d}}{\mathrm{d}q_1} \cdots \frac{\mathrm{d}}{\mathrm{d}q_\ell} \log \left\langle \exp\left[\sum_{i=1}^{\ell} q_i\, \omega(\mathbf{g}_i, T) \right] \right\rangle$$

Show that these cumulants all amount to

$$C(\Omega(\mathbf{g}_1), \ldots, \Omega(\mathbf{g}_\ell)) = \frac{1}{T} \frac{\mathrm{d}^\ell}{\mathrm{d}q^\ell} \log \langle \exp\left[q\, \omega(\mathbf{0}, T) \right] \rangle$$

$\star$ d) Generalize the finding of (c) to the joint cumulants with other observables.