Stochastic Processes **Tutorial 4**

3 May 2018 Cumulants of Markov Processes

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Exercise 1 *Gauge Invariance of Antisymmetric Observables*

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

(a) Show that $\Omega(\vec{g}) := (i \to j) \mapsto \omega_j^i(\vec{g}) = \log \frac{w_j^i\, g_i}{w_i^j\, g_j}$ is an antisymmetric observable, irrespective of the choice of $\vec{g}$.

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

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

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

Show that these cumulants all amount to

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

(optional) Generalize the finding of (c) to the joint cumulants with other observables.

Exercise 2 *Kolmogorov's Cycle Criterion*

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

$$\mathring{\omega}_\alpha = \sum_{i \to j \in \zeta_\alpha} \omega_j^i = 0 \quad \text{for all cycles } \zeta_\alpha$$

We proof this statement in three steps.

(a) Show that the criterion can be relaxed: It is sufficient when the values $\mathring{\omega}_\alpha$ 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 $g_i = w_i^j g_j / w_j^i$ 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 $i \in \{1, \ldots, N\}$. 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?

Exercise 3 *Cumulants for the Kinesin Molecular Motor Model*

The Kinesin Molecular Motor performs steps along a microtubule (*displacement current* $\mathcal{D}$) on expense of hydrolyzing ATP into ADP (*chemical current* $\mathcal{C}$). In the lecture we saw that its motion can be modeled by dynamically reversible Markov model with four states, where transitions between all states are possible except for the transitions $1 \leftrightarrow 4$. In this model the observables $\Omega_{\mathcal{D}}$ and $\Omega_{\mathcal{C}}$ take the following form

$$\Omega_{\mathcal{D}} := \begin{cases} (3 \to 2) & \mapsto \quad 1 \\ (2 \to 3) & \mapsto \ -1 \\ (i \to j) & \mapsto \quad 0 \quad \text{else} \end{cases} \qquad \text{and} \qquad \Omega_{\mathcal{C}} := \begin{cases} (2 \to 1) & \mapsto \quad 1 \\ (1 \to 2) & \mapsto \ -1 \\ (3 \to 4) & \mapsto \quad 1 \\ (4 \to 3) & \mapsto \ -1 \\ (i \to j) & \mapsto \quad 0 \quad \text{else}\,. \end{cases}$$

We explore different representations of the covariance of the displacement and chemical current.

(a) Show that for every pair (Φ, Ψ) of antisymmetric variables the covariance $C(\Phi, \Psi)$ can be expressed in terms of the circulations $\mathring{\varphi}_\delta$ and $\mathring{\psi}_\eta$ for the fundamental cycles selected by the chords δ and η and the covariance $C(\delta, \eta)$ of the associated chord variables. For a system with B chords this decomposition reads

$$C(\Phi, \Psi) = \sum_{\delta=1}^{B} \sum_{\eta=1}^{B} C(\delta, \eta)\, \mathring{\varphi}_\delta\, \mathring{\psi}_\eta\,. \tag{2a}$$

Provide to that end the appropriate definitions of $\mathring{\varphi}_\delta$, $\mathring{\psi}_\eta$, and $C(\delta, \eta)$.

(b) Consider now the model for the Kinesin Molecular Motor. Select the chords $\alpha := (1 \to 2)$ and $\beta := (2 \to 3)$, and show that Eq. (2a) will then taken the form

$$C(\mathcal{D}, \mathcal{C}) = 2\, C(\alpha, \beta) - C(\beta, \beta) \tag{2b}$$

(c) Select the chords $\alpha := (1 \to 2)$ and $\gamma := (3 \to 4)$, and show that Eq. (2a) will then taken the form

$$C(\mathcal{D}, \mathcal{C}) = C(\alpha, \alpha) - C(\gamma, \gamma) \tag{2c}$$

Hint: Watch out, the values $\mathring{\varphi}_\alpha$ and $\mathring{\psi}_\alpha$ depend on the choice of the chords!

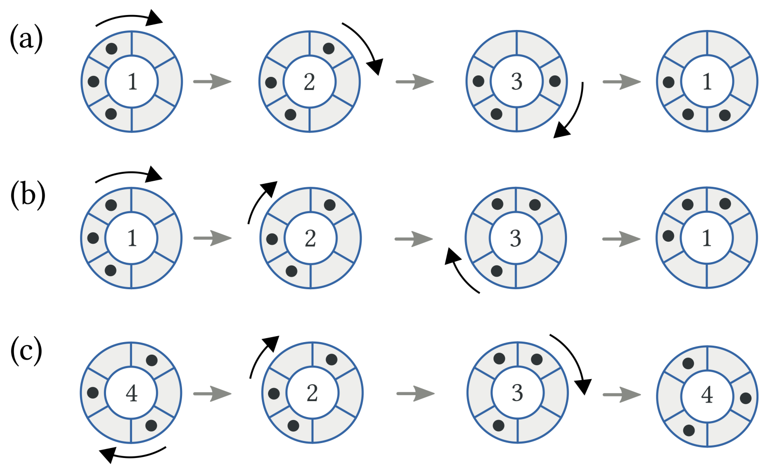
(d) In order to understand the relation between these representations, we consider the representation of the edge observable γ (i.e., the observable that counts the net number of traversals of the edge $3 \to 4$) in the representation where α and β are chords. Verify that

$$C(\gamma, \gamma) = C(\alpha, \alpha) - 2\, C(\alpha, \beta) + C(\beta, \beta)\,.$$

How does this help to clarify the relation between Eq. (2b) and (2c)?

Exercise 4 *Simple Exclusion Process for 3 Particles on 6 Sites*

In the lecture we discussed the simple exclusion process for 3 partices and 6 sites. Periodic boundary conditions are used to identify states that only differ by rotation. For instance, 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.



In this exercise we 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 $\det\left(\hat{\mathbb{W}}_{\mathcal{D}} - \lambda\, \mathbb{I}_4\right)$ 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 $\hat{\mathbb{W}}(\vec{q})$ 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.