Blatt 3. Markov Processes 1

The sign indicates exercises whose solution might require additional study and some effort.
Please choose to work either on either 3.4.d), 3.4.e) or 3.5.c)

Problems

3.1. Stationary solutions for Markov processes

A stochastic process is called *stationary* when its moments are not affected by a shift in time.

a) Consider the biased random walk discussed in Exercise 2.1. Is this a stationary process?

b) Now we consider a random walk on $\mathbb{Z}$ with position-dependent probabilities

$$\begin{aligned} r_j &= K\,\mathrm{e}^{-\beta j} \qquad \text{to go from site } j \text{ to } j+1, \\ l_j &= K\,\mathrm{e}^{\beta j} \qquad \text{to go from site } j \text{ to } j-1. \end{aligned}$$

In these expressions β and K take constant values in $\mathbb{R}^+$ and $[0,1]$, respectively.

Let $X_t \in \mathbb{Z}$ be the position of a random walker at time t. Verify that the probability to find the walker at time t at lattice site $j \in \mathbb{Z}$ is a Markov process.

c) This process admits an equilibrium state $p_j^{\mathrm{eq}}, j \in \mathbb{Z}$ that obeys

$$r_j\, p_j^{\mathrm{eq}} = l_{j+1}\, p_{j+1}^{\mathrm{eq}} \qquad \text{for all} \quad j \in \mathbb{Z}\,.$$

Clearly, it defines a stationary Markov process.

d) Determine the probability distribution $p_j^{\mathrm{eq}}, j \in \mathbb{Z}$ and its cumulants.

3.2. Cycle Representation of Stationary States

Proof the following statements about stationary states of Markov processes on a finite graph $\mathcal{G}$.

a) Equilibrium states are stationary states.
Hint: Equilibrium states obey detailed balance $w_j^i\, p_i = w_i^j\, p_j$ for all pairs i, j of states.

b) The time evolution of the probability p_k to find a realization of a Markov process in state k evolves according to

$$\dot{p}_k = \sum_{i, i\neq k} J_k^i \qquad \text{with} \quad J_k^i = w_k^i\, p_i - w_i^k\, p_k\,. \tag{3.1a}$$

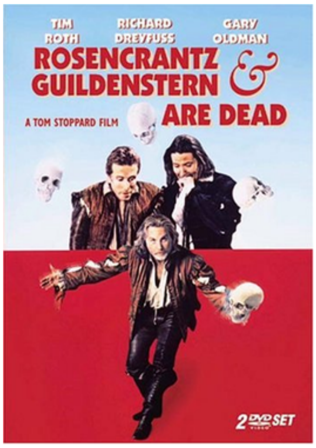
c) In a steady state the currents can be written as superpostions of cycle currents

$$J^i_k = \sum_{\alpha \in \mathsf{X}} J_\alpha \, \Theta_\alpha(i \to k) \qquad \text{with} \quad \Theta_\alpha(i \to k) = \begin{cases} 1 & \text{if} \quad i \to k \in \zeta_\alpha \\ -1 & \text{if} \quad k \to i \in \zeta_\alpha \\ 0 & \text{else} \end{cases} \tag{3.1b}$$

where X is a set of chords for the graph $\mathcal{G}$.
Hint: What happens when $i \to k$ is a chord? Use Kirchhoffs law to determine what happens on the other edges of the graph.

d) The time derivative $\dot{p}_k$ vanishes when inserting Equation (3.1b) into the right-hand side of Equation (3.1a).

3.3. Rosencrantz Coin Tossing



The Tom Stoppard movie Rosencrantz & Guildenstern are Dead starts with a prolonged reflection on information theory and negative entropy events; exemplified by an unusual sequence of outcomes of a coin tossing experiment. We repeat Rosenkrantz experiment of coin flipping: Initially, we see head. We flip again when we see head. However, once we encounter tail we are happy, stop, and reply tail on any further inquiry. Let the coin flip be biased with a probability p to encounter head.

a) Implement the expriment in a Sage or Python script, and explore the probability distribution of the number of tosses till one first encounters tail.

b) Sketch the graph for this Markov process and mark the transfer probabilities.
Do we have dynamical reversibility? Do we have an absorbing state?

c) Write down the transition matrix and determine its eigenvalues. For a normal random walk the entries of the columns of the transition matrix add to zero and that there is a zero eigenvalue. What is different here?

Determine the left and right eigenvectors $\langle 1|$ and $|1\rangle$ of the steady state, and the eigenvectors $\langle d|$ and $|d\rangle$ representing transients. In this notation d represents the probability of decay for the transient state.

d) Show that the probability distribution $\mathbf{P}(N) = |N\rangle$ after N flips takes the form

$$|N\rangle = p^N \; |H\rangle + (1 - p^N) \; |T\rangle \qquad \text{with} \quad |H\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |T\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

3.4. Reaction with two decay channels

Let I be a substance that decays into the stable substances A and B with a rates a and b, respectively.

a) Sketch the graph for this Markov process and mark the transition rates.

b) Write down the transition matrix. Find its eigenvalues, the eigenvectors $|A\rangle$, $|B\rangle$ and $\langle A|$, $\langle B|$ of the steady states, and the eigenvectors $|d\rangle$, $\langle d|$ representing transients that decay with a rate d.

c) Represent the state of the system as

$$\mathbf{P}(t) = |t\rangle = \rho_A(t)\ |A\rangle + \rho_B(t)\ |B\rangle + \rho_I(t)\ |I\rangle \quad \text{with} \quad |I\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} ,$$

and determine the time evolution for a sample that initially contains only substance I.

$\star$ d) Plot the abundance of the species in a plot, where the filled area under $p_A(t)$ shows the fraction of the population in state A, another filled area between the curves $p_A(t)$ and $p_A(t) + p_I(t)$ indicates the fraction of the population in state I, and the filled area between $p_A(t)+p_I(t)$ and 1 indicates the fraction of the population in state B. Let the initial condition be $p_I(0) = 1$. How does the plot change upon varying the rates a and b. One of the rates, let us say a, can be absorbed into the time constant by introducing the dimensionless time at. How does the shape of the graph depend then on the dimensionless parameter b/a?

$\star$ e) Repeat the analysis for the decay of an initial substance I to B with an intermediary product A, *i.e.,* I decays to A with rate a, and then A decays to B with rate b.

3.5. Three interacting particles on four sites (Part 1)

We consider a system with four binding sites on a ring. 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) Sketch the graph for this Markov process and mark the transition rates.
Do we have dynamical reversibility? Do we have an absorbing state?

b) Write down the transition matrix W.

c) Write a simulation that follows the dynamics of the system, and build an animation of the evolution.
Instruction: For simplicity we perform the simulation for the time discrete model where d, u, r and $l = 1 - r$ are probabilites. The simulation is driven by randomly in each time step a transition and accepting the step when the probability associated to the step is larger than a random number that is uniformly sampled in $[0, 1]$ in order to take the decision.