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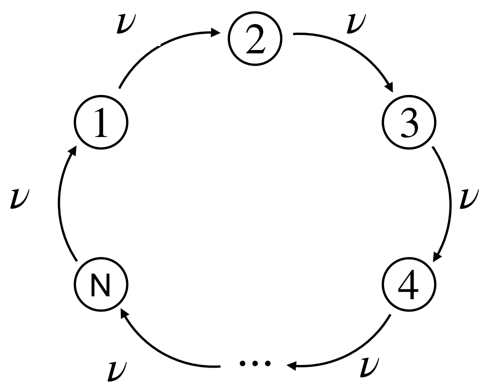
Nonequilibrium Field Theories and Stochastic Dynamics
Sheet 3

Exercise 9 – Poisson Process on a Ring

In this exercise, we will find out under which conditions probability currents do not change the probability distribution in a stochastic system and how the concept of irreversibility and entropy production is connected to this.



We consider a continuous-time Markov process on a ring of N discrete states. Transitions occur only from $i \to i+1$ mod N at constant rate ν. This is a minimal model of a non-equilibrium steady state with persistent probability currents.

a) The probability distribution is then a vector $\mathbf{p}(t) \in [0,1]^N$ with N entries between 0 and 1. It evolves according to the master equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p}(t) = \mathbf{Q} \cdot \mathbf{p}(t), \tag{1}$$

Write down the $\mathbf{Q}$-matrix for the Poisson process on a ring. Find its eigenvalues and determine the stationary state $\mathbf{p}_{\mathrm{st}}$. What kind of distribution do you find? Give a heuristic argument for your finding. Does $\mathbf{p}_{\mathrm{st}}$ obey detailed balance?

Hint: $\boldsymbol{p}_{st}$ is the eigenvector to the eigenvalue zero. Furthermore, you might find this eigenvector ansatz useful: $\boldsymbol{p}_\omega = (1, \omega, \omega^2, ..., \omega^{N-1})^T$.

b) In the lecture you have seen that the probability current from site j to i is given by

$$J_{ij}(t) = \omega_{ij}\, p_j(t) - \omega_{ji}\, p_i(t)\,. \tag{2}$$

Calculate $J_{i+1,i}$ for the stationary distribution. How does this system differ from a thermodynamic system?

c) On a circle, we can assign each site, e.g. the k^{th}, a complex number, $e^{2\pi ik/N} =: e^{i\theta_k}$, with the unique phase value $\theta_k = 2\pi k/N$. Give an interpretation of the following quantity $\phi(t)$

$$\phi(t) := \langle e^{i\theta_k} \rangle(t) = \sum_{k=0}^{N-1} e^{2\pi ik/N}\, p_k(t)\,. \tag{3}$$

Hint: To get some intuition you can use $p_k(t) = \delta_{k,n(t)}$, where $n(t)$ in the limit for large N can be seen as quasi-continuous: $n(t) = \nu t$. Determine the time evolution of $\phi(t)$ and interpret the result for large N.

Hint: Expand your result to second order in $1/N$. What do the terms mean? Remember the Taylor expansion series of the exponential.

d) Knowing whether a process is reversible or irreversible helps us understand how energy is converted, which is key for e.g. designing efficient systems. For this reason we introduce the entropy production rate:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S} = \sum_{i,j} p_j Q_{ij} \ln\left(\frac{Q_{ij}p_j}{Q_{ji}p_i}\right) . \tag{4}$$

This basically quantifies the *irreversibility* of a process. [1]

What is the value of the entropy production if a system is in detailed balance? And what does this tell us about the reversibility of such a process?

e) We now introduce backward jumps with a rate ϵ (meaning $Q_{i-1,i} = \epsilon$). Does this change our steady state solution?

Calculate the entropy production for this adapted process. Take the limit $\epsilon \to 0$ of the obtained result and interpret it.

f) How does a typical trajectory of a single particle look like? Why doesn't this contradict the ensemble statistics described by the probability distribution? Describe in words, you do not have to do the numerics.

Exercise 10 – Markov processes with infinite state spaces

In the lecture we have discussed some important general properties of Markov processes that can be derived from the transition rate matrix $\boldsymbol{Q}$. Arguably the most important result was that irreducible Markov processes always have a unique stationary state $\boldsymbol{\pi}$. But it was also stated that these general statements might not hold anymore as we move to a Markov process with a countably infinite number of states.[2]

In this exercise we want to analyze two simple stochastic processes with $N+1$ possible states and see if and how things can go wrong as we take $N \to \infty$.

a) Let us first consider a symmetric random walk on a one-dimensional lattice with hopping rates $\varepsilon_+ = \varepsilon_- = \varepsilon$. Assume that the position $X(t)$ of the random walker is confined to $n \in \{0, \dots, N\}$, i. e., there are reflective boundaries at positions $n = 0$ and $n = N$, such that the walker can only hop forward at the one end, or backward at the other. Write down the master equation for $p_n(t) = \text{Prob}\{X(t) = n\}$, including the proper boundary terms for $p_0(t)$ and $p_N(t)$, and give the transition rate matrix $\boldsymbol{Q}_N$. Why can we set $\varepsilon = 1$ throughout the rest of the problem?

b) Show that for any value of $N \in \mathbb{N}^+$ this process obeys detailed balance and give the stationary probability distribution $\pi_n = \text{Prob}\{X(t \to \infty) = n\}$.

c) Given its simplicity, one might think that the symmetric random walk we defined above also has a well-defined limit if we increase the system size. Considering the stationary state, describe the problem we face as we take the limit $N \to \infty$.

Another way to see that a problem emerges at large N is by applying the theorem of Perron and Frobenius. What can you say, heuristically, about the number of eigenvalues λ of $\boldsymbol{Q}_N$ that are close to zero, as we take $N \to \infty$?

Note: We define the eigenvalues here with a negative sign, i. e., $\boldsymbol{Q}_N\boldsymbol{\phi} = -\lambda\boldsymbol{\phi}$.

d) We want to be more precise about the number and location of the eigenvalues of the transition rate matrix. Given its particular structure, we can analyze the eigenvalues of $\boldsymbol{Q}_N$ for general N by studying its characteristic polynomial Δ_{N+1} (we use the total number of states as subscript, i. e.the dimensions of $\boldsymbol{Q}_N$)

$$\Delta_{N+1}(\lambda) \coloneqq \det\left(\boldsymbol{Q}_N + \lambda\mathbf{1}\right) = 0 . \tag{5}$$

Derive the following expression for the polynomial:

$$\Delta_{N+1}(\lambda) = (\lambda - 1)\tilde{\Delta}_N - \tilde{\Delta}_{N-1} , \tag{6}$$

[1] The logarithmic terms measure the difference between the forward ($Q_{ij}p_j$) and the backwards rate ($Q_{ji}p_i$), which determine how irreversible the reaction between the state i and j is. The logarithms are then weighted by p_jQ_{ij}, which measures how likely the respective transition between state i and j will occur. The structure of the entropy production rate is reminiscent to the Kullback–Leibler divergence, which describes the 'distance' of a true distribution from an approximate distribution.

[2] If we think about *uncountably* infinite state spaces, we are essentially describing a continuous state space, for which we need entirely different approaches. We will learn about those in the course of the lecture.

where $\tilde{\Delta}_m(\lambda)$ is the characteristic polynomial of a different matrix (which one?). Show that $\tilde{\Delta}_m(\lambda)$ obeys the following recurrence relation (you do not need to solve it):

$$\begin{aligned}\tilde{\Delta}_m(\lambda) &= (\lambda-2)\tilde{\Delta}_{m-1}(\lambda) - \tilde{\Delta}_{m-2}(\lambda)\\ \tilde{\Delta}_1(\lambda) &= \lambda - 1\\ \tilde{\Delta}_0(\lambda) &= 1\end{aligned} \tag{7}$$

e) One can show that the non-zero eigenvalues of $\boldsymbol{Q}_N$ lie in the open interval $\lambda \in (0,4)$ and are given by the solutions to this equation:

$$\left(\lambda - 2 + \sqrt{\lambda(\lambda-4)}\right)^{N+1} = \left(\lambda - 2 - \sqrt{\lambda(\lambda-4)}\right)^{N+1} \tag{8}$$

Show that the solutions to this equation are non-degenerate and grow arbitrarily close to zero as we increase N. Argue why this results in the breakdown of the steady state solution for $N \to \infty$. Plot the ten lowest eigenvalues for values of N between 10 and 100 to visualize what you have found.

Hint: If you cannot solve the equation, calculate/plot the eigenvalues numerically and observe a trend. Looking at the equation, try to argue if it is possible to have an eigenvalue with multiplicity greater than one. If not, what does this mean for the zero eigenvalue as we take $N \to \infty$?

f) Lastly, we want to repeat the analysis for a slightly different system, where the limit $N \to \infty$ preserves the steady state. Imagine the following one-step process: A source emits particles X at a constant rate ε_+ ($\emptyset \to X$), but they also decay with a rate ε_- ($X \to \emptyset$). In a biological context, we could also think of a large reservoir of molecules A, producing molecules X. We denote the number of particles at a given time by $X(t)$ and constrain its values to $n \in \{0, \dots, N\}$ (e. g.because there is a fixed carrying capacity of X-particles in the environment).

Write down the master equation describing the dynamics of $p_n(t)$ and the transition rate matrix $\boldsymbol{Q}_N$. Assume for simplicity that $\varepsilon_+ = \varepsilon_- =: \varepsilon$. Derive another recurrence relation of the form of Eqs. (6) and (7). (Again, you do not need to solve it.)

Hint: It might help to reverse the usual ordering of the states for obtaining the recurrence relation.

g) Lastly, argue based on the transition rate matrix and the Perron-Frobenius theorem why this system does not have the same problem as the symmetric random walk (eigenvalues moving closer and closer to zero). Compute the ten lowest eigenvalues numerically and plot them for N between 10 and 100. What do you observe? Does this system still allow for a (unique) steady state in the limit $N \to \infty$? What would you expect to happen for the random walk if we make it *asymmetric*, i. e., change the ratio of $\varepsilon_+/\varepsilon_-$?

Hint: Computing the eigenvalues can be done, for instance, in Numpy. To define matrices of a certain type, have a look at the function `numpy.diagflat`, and at `numpy.linalg.eig` to find their eigenvalues.

Your solutions should be handed in by uploading them to Moodle by **Wednesday, 21$^{\text{th}}$ May 2025, 10:00 am**.