SAMPLE SOLUTIONS EXERCISE 3

EXERCISE 3.1: VECTOR NOTATION AND LIOUVILLE OPERATOR (6P)

Consider a continuous-time Markov process (see lecture notes) with the master equation

$$\dot{P}_c(t) = \sum_{c'} P_{c'}(t) w_{c' \to c} - P_c(t) \sum_{c'} w_{c \to c'}.$$

(a) Prove that the matrix elements of the Liouville operator $\mathcal{L}$ are given by (3P)

$$\langle c' | \mathcal{L} | c \rangle \;=\; -w_{c \to c'} + \delta_{c,c'} \sum_{c''} w_{c \to c''}$$

(b) Consider a system with three configurations $1, 2, 3$ with the rates

$$w_{1\to 2} = 1\,, \quad w_{2\to 1} = \frac{1}{2}\,, \quad w_{2\to 3} = 1\,, \quad w_{3\to 1} = 5\,,$$

in units of $1/\text{time}$ (all other rates are zero). Determine the matrix of the Liouville operator. (1P)

(c) Determine the so-called zero vectors, i.e., the left and right eigenvectors to the eigenvalue zero. (1P)

(d) Normalize the right zero vector in order to interpret it as a probability distribution. Why are the components of the left and the right eigenvector numerically different? (1P)

SAMPLE SOLUTION

(a) Starting with $|\dot{P}_t\rangle = -\mathcal{L}|P_t\rangle$ we first insert a $\mathbb{1} = \sum_{c''} |c''\rangle\langle c''|$: (1P)

$$|\dot{P}_t\rangle = -\sum_{c''} \mathcal{L}|c''\rangle\langle c''|P_t\rangle$$

Applying the bra vector $\langle c'|$ for some arbitrarily chosen configuration c' from the left, this turns into

$$\langle c'|\dot{P}_t\rangle = -\sum_{c''} \langle c'|\mathcal{L}|c''\rangle\langle c''|P_t\rangle \quad \Rightarrow \quad \dot{P}_{c'}(t) = -\sum_{c''} \mathcal{L}_{c',c''}\, P_{c''}(t).$$

Inserting the master equation $\dot{P}_{c'}(t) = \sum_{c''} P_{c''}(t) w_{c''\to c'} - P_{c'}(t) \sum_{c''} w_{c'\to c''}$ on the left side, we get (1P)

$$\sum_{c''} P_{c''}(t) w_{c''\to c'} - P_{c'}(t) \sum_{c''} w_{c'\to c''} \;=\; -\sum_{c''} \mathcal{L}_{c',c''}\, P_{c''}(t)\,.$$

This equation holds for any valid probability distribution $P_c(t)$. Hence all what remains to be done is to compare the coefficients of this equation. This is carried out most easily by partially differentiating with respect to $P_c(t)$, and using that $\frac{\partial P_{c'}(t)}{\partial P_c(t)} = \delta_{c',c}$ this yields

$$w_{c \to c'} - \delta_{c,c'} \sum_{c''} w_{c \to c''} \;=\; -\mathcal{L}_{c',c}$$

which completes the proof. (1P)

(b) The matrix reads (1P)

$$\mathcal{L} = \begin{pmatrix} 1 & -1/2 & -5 \\ -1 & 3/2 & 0 \\ 0 & -1 & 5 \end{pmatrix}$$

(c) Because of probability conservation, we always have $\langle \Sigma | \mathcal{L} = 0$, where $\langle \sigma |$ is a row vector containing only 1s, i.e., $\langle \Sigma | = (1, 1, 1)$. Hence it is a left eigenvector to the eigenvalue zero. The right eigenvector $\mathcal{L}|\phi\rangle = 0$ can be found by solving a linear system of equations or asking *Mathematica®* ; it reads

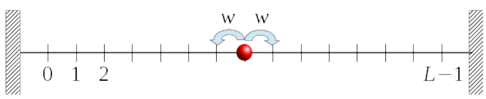
$$|\phi\rangle = \begin{pmatrix} 15 \\ 10 \\ 2 \end{pmatrix}$$

(d) To normalize the right eigenvector, the sum of all components should be equal to 1. This can be achieved by dividing the unnormalized vector given above by 27:

$$|\phi\rangle = \frac{1}{27} \begin{pmatrix} 15 \\ 10 \\ 2 \end{pmatrix}$$

Exercise 3.2: One-dimensional random walk **(6P)**

Consider a particle on a one-dimensional chain with L sites with closed ends performing a symmetric random walk at a constant rate w. Let us enumerate the sites with the index $j = 0, \ldots, L-1$.



(a) Find the $L \times L$ matrix of the Liouville operator $\mathcal{L}$ in the configuration basis. (1P)

(b) Consider the eigenvalue problem $\mathcal{L}|\psi_n\rangle = \lambda_n |\psi_n\rangle$ and show that the ansatz

$$(\psi_n)_j = \langle c_j | \psi_n \rangle = A e^{i k_n j} + B e^{-i k_n j}$$

evaluated in the bulk of the chain leads to the dispersion relation $\lambda_n = 4w \sin^2 \frac{k_n}{2}$. (Here $\langle c_j |$ denote the canonical basis vectors). (2P)

(c) Take the boundary conditions (the first and the last line of the matrix) into account in order to determine all eigenvectors and eigenvalues of $\mathcal{L}$. (2P)

(d) What is the longest typical time scale occurring in the dynamics? How does it depend on L? (1P)

Sample Solution

(a) This is just a variant of the matrix given in the lecture notes:

$$\mathcal{L} = \begin{pmatrix} w & -w & & & & \\ -w & 2w & -w & & & \\ & -w & 2w & -w & & \\ & & \cdots & \cdots & \cdots & \\ & & & \cdots & \cdots & \cdots \\ & & & & -w & w \end{pmatrix}$$

(b) Inserting the ansatz into the bulk equations (all lines of the matrix except for the first and the last one) yields

$$w\Big[A\Big(-e^{ik(j-1)}+2e^{ikj}-e^{ik(j+1)}\Big)+B\Big(-e^{-ik(j-1)}+2e^{-ikj}-e^{-ik(j+1)}\Big)\Big] = \lambda(Ae^{ikj}+Be^{-ikj})$$

This can be rewritten as

$$w\Big[A\Big(-e^{-ik}+2-e^{ik}\Big)e^{ikj}+B\Big(-e^{+ik}+2-e^{-ik}\Big)e^{-ikj}\Big] = \lambda(Ae^{ikj}+Be^{-ikj})$$

This equation has to hold for any A, B and for all j. This requires the terms proportional to A and B to cancel separately, leading to the dispersion relation

$$\lambda = w(-e^{-ik}+2-e^{ik}) = 4w\,\sin^2(k/2). \qquad (1)$$

(c) The remaining unknowns A, B, k can be determined from the boundary equations and the normalization condition. The left boundary equation (first line with the above ansatz) reads

$$w\Big[A\Big(1-e^{ik}\Big)+B\Big(1-e^{-ik}\Big)\Big] = \lambda(A+B)$$

Combined with Eq. (1) the left boundary condition fixes the relative phase between A and B:

$$A = Be^{ik}$$

So we may choose e.g. $A = \frac{1}{2}e^{ik/2}$ and $B = \frac{1}{2}e^{-ik/2}$.
The right boundary equation (last line of the matrix with the ansatz inserted) is given by

$$w\Big[A\Big(1-e^{-ik}\Big)e^{ik(L-1)}+B\Big(1-e^{ik}\Big)e^{-ik(L-1)}\Big] = \lambda_k\Big(Ae^{ik(L-1)}+Be^{-ik(L-1)}\Big).$$

Inserting λ and A it reduces to

$$-4\sin(k/2)\sin(kL) = 0$$

with the quantized solutions $k_n = n\pi/L$ with $n = 0, \ldots, L-1$. This leads to the final solution

$$(\psi_k)_j = \langle c_j|\psi_k\rangle = \tilde{A}\cos\Big(\frac{n\pi(j+1/2)}{L}\Big), \qquad \lambda_n = 4w\sin^2\Big(\frac{n\pi}{2L}\Big)$$

with some arbitrary amplitude $\tilde{A}$.

If you like you may check these results with *Mathematica®* as follows:

```
L = 5; w = 1;
Einsvektor = Table[1, L];
Liouville =
w*Table[-KroneckerDelta[i - 1, j] - KroneckerDelta[i + 1, j],
        {i, L}, {j, L}];
Liouville -= DiagonalMatrix[Einsvektor.Liouville];
Liouville // MatrixForm

lambda[n_] := 4 w Sin[n Pi/2/L]^2;
eigenvector[n_] := Table[Cos[n Pi (j + 1/2)/L], {j, 0, L - 1}];
Table[Liouville.eigenvector[n] - lambda[n]*eigenvector[n],
      {n, 0,  L - 1}] // FullSimplify
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(d) The longest time scale is the reciprocal of the smallest non-vanishing eigenvalue

$$T = \frac{1}{\lambda_1} = \frac{1}{4w\sin^2\left(\frac{\pi}{2L}\right)} \approx \frac{L^2}{\pi^2 w}.$$

(Σ = 12P)