Stochastic Processes (hints for solution) — Tutorial 3

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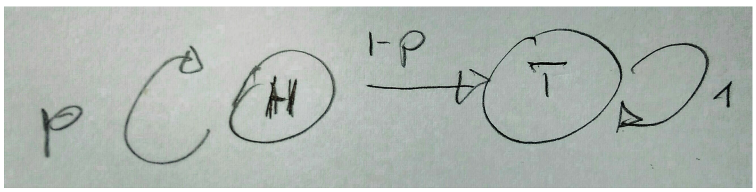
Universität Leipzig
Institut für Theoretische Physik
Jürgen Vollmer

Exercise 2 *Coin Tossing*

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) Sketch the graph for this Markov process and mark the transfer probabilities.



Do we have dynamical reversibility?
No – one can go from $H \to T$ and not backwards

Do we have an absorbing state?
Yes – state T

(b) Write down the transition matrix and determine its eigenvalues.

$$\mathtt{W} = \begin{pmatrix} p & 0 \\ 1-p & 1 \end{pmatrix}$$

with eigenvalues p and 1.
In the lecture we showed that the entries of the columns of the transition matrix add to zero and that there is a zero eigenvalue. What is different here?
These findings refer to time-continuous Markov processes, where the transfer matrix describes the time evolution of the derivative of the probabilities. In this exercise we are dealing with a time-discrete problem.

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.

In the present case the transient state decays with probability p. Hence,

$$\langle p| = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad \langle 1| = \begin{pmatrix} 1 & 1 \end{pmatrix}, \quad |p\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Note that these vectors are orthonormal $\langle i|j\rangle = \delta_{ij}$ for $i, j \in \{p, 1\}$
and complete $|p\rangle\langle p| + |1\rangle\langle 1| = \mathbb{I}_2$ where $\mathbb{I}_2$ is the 2×2 unit matrix.

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

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

We use the time evolution operator and the eigenvalue representation of $\mathbb{I}_2$ to determine the probability distribution $|N\rangle$ obtained after N flips when starting with the initial distribution $|H\rangle$:

$$|N\rangle = \mathbb{I}_2 \mathbb{W}^N |0\rangle = |p\rangle \langle p| \mathbb{W}^N |H\rangle + |1\rangle \langle 1| \mathbb{W}^N |H\rangle = |p\rangle\, p^N \langle p|H\rangle + |1\rangle \langle 1|H\rangle = p^N |p\rangle + |1\rangle$$

In the last step we used that

$$\langle p|H\rangle = (1,0) \begin{pmatrix}1\\0\end{pmatrix} = 1 \qquad \text{and} \qquad \langle 1|H\rangle = (1,1) \begin{pmatrix}1\\0\end{pmatrix} = 1$$

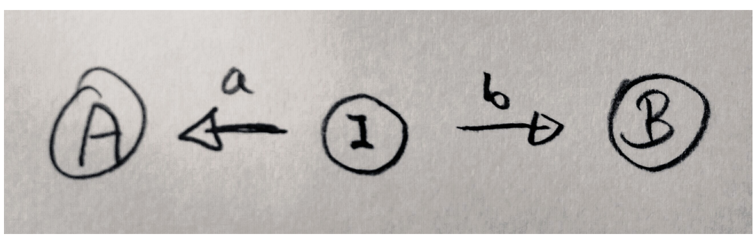
Hence, we find

$$|N\rangle = p^N \begin{pmatrix}1\\-1\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}p^N\\1-p^N\end{pmatrix} = p^N\ |H\rangle + (1-p^N)\ |T\rangle\ .$$

Exercise 3 *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.

$$\mathtt{W} = \begin{pmatrix} 0 & a & 0 \\ 0 & -a-b & 0 \\ 0 & b & 0 \end{pmatrix}$$

Find its eigenvalues,
— the eigenvalues are 0, 0 and $-(a+b)$ —
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.
Here, the decay rate d is $d = -a-b$ such that

$$|A\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix} , \quad |B\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix} , \qquad |-a-b\rangle = \frac{1}{a+b} \begin{pmatrix}-a\\a+b\\-b\end{pmatrix}$$

$$\langle A| = \begin{pmatrix}1, & \frac{a}{a+b}, & 0\end{pmatrix} , \quad \langle B| = \begin{pmatrix}0, & \frac{b}{a+b}, & 1\end{pmatrix} , \quad \langle -a-b| = \begin{pmatrix}0, & 1, & 0\end{pmatrix} .$$

Due to the degeneray of the eigenvalue 0 the choice of the eigenvectors is not unique. For the present choice the eigenvectors are orthonormal and complete.
Note, that the left eigenvector $(1,1,1)$ is also present; after all $\langle A| + \langle B| = (1,1,1)$ is also an eigenvector with zero eigenvalue.

(c) Represent the state of the system as

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

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

$$\langle A|I\rangle = \frac{a}{a+b}\,, \qquad \langle -a-b|I\rangle = 1\,, \qquad \langle B|I\rangle = \frac{b}{a+b}$$

Moreover, the time evolution of the projection of a state $\vec{P}(t) = |t\rangle$ to an eigenvector $|\lambda\rangle$ with eigenvalue λ amounts to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\lambda|t\rangle = \langle\lambda|\,\mathbb{W}\,|t\rangle = \lambda\langle A|t\rangle \quad \Rightarrow \langle\lambda|t\rangle = \mathrm{e}^{\lambda\,t}\ \langle\lambda|0\rangle$$

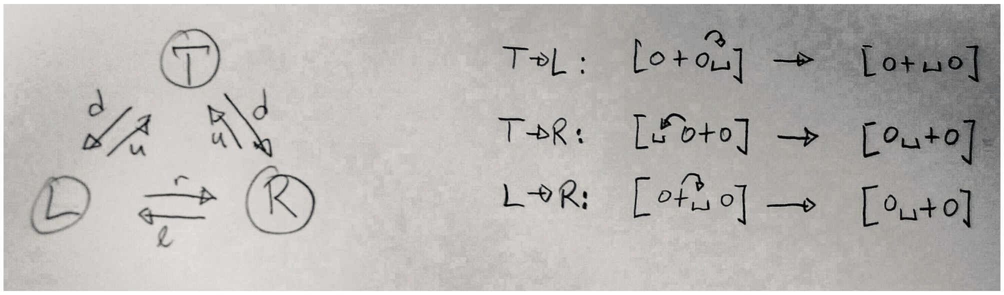
where $|0\rangle$ is the initial condition for $|t\rangle$. Altogether, we thus obtain for $|t\rangle = \vec{P}(t)$ with initial condition $\vec{P}(0) = |I\rangle$,

$$\begin{aligned}
|t\rangle &= |A\rangle\ \langle A|t\rangle + |B\rangle\ \langle B|t\rangle + |-a-b\rangle\ \langle -a-b|t\rangle \\
&= |A\rangle\ \langle A|I\rangle + |B\rangle\ \langle B|I\rangle + |-a-b\rangle\ \mathrm{e}^{-(a+b)\,t}\ \langle -a-b|I\rangle \\
&= \frac{a}{a+b}\begin{pmatrix}1\\0\\0\end{pmatrix} + \frac{b}{a+b}\begin{pmatrix}0\\0\\1\end{pmatrix} + \frac{\mathrm{e}^{-(a+b)\,t}}{a+b}\begin{pmatrix}-a\\a+b\\-b\end{pmatrix} \\
&= \frac{a}{a+b}\ \left(1-\mathrm{e}^{-(a+b)\,t}\right)\ |A\rangle + \frac{b}{a+b}\ \left(1-\mathrm{e}^{-(a+b)\,t}\right)\ |B\rangle + \mathrm{e}^{-(a+b)\,t}\ |I\rangle
\end{aligned}$$

Exercise 4 *Three interacting particles on four sites*

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?
The dynamics is dynamically reversible and there are no absorbing states.

(b) Write down the transition matrix W

$$\mathbb{W} = \begin{pmatrix} -u-r & d & l \\ u & -2d & u \\ r & d & -u-l \end{pmatrix}$$

and the skewed transition matrix $\hat{\mathrm{W}}$ 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 $w^i_j\, \mathrm{e}^{s\,\omega^i_j}$.

$$\hat{\mathbb{W}} = \begin{pmatrix} -u-r & d\,\mathrm{e}^{s\omega^T_L} & l\,\mathrm{e}^{s\omega^R_L} \\ u\,\mathrm{e}^{-s\omega^T_L} & -2d & u\,\mathrm{e}^{s\omega^T_R} \\ r\,\mathrm{e}^{-s\omega^R_L} & d\,\mathrm{e}^{-s\omega^T_R} & -u-l \end{pmatrix}$$

(c) 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)).
For $P(\lambda; s) = \det\left(\hat{\mathbb{W}} - \lambda\,\mathbb{I}_3\right)$ one finds the coefficients

$$\begin{aligned}
a_3 &= -1 \\
a_2 &= -2u - 2d - r - l \\
a_1 &= -((u+r)\,2d - ud) - ((u+r)\,(u+l) - lr) - (2d\,(u+l) - ud) \\
&= -(2d+u)\,(u+r+l) \\
a_0 &= -(u+r)\,2d\,(u+l) + dur\,\mathrm{e}^{s\bar{\omega}} + dul\,\mathrm{e}^{-s\bar{\omega}} + (u+r)\,du + 2d\,rl + (u+l)\,ud \\
&= ud\,\left(r\,\mathrm{e}^{s\bar{\omega}} + l\,\mathrm{e}^{-s\bar{\omega}} - 2\right)
\end{aligned}$$

Note that $a_N = (-1)^N$, $a_{N-1} = (-1)^{N-1}\ \mathrm{Tr}\,\hat{\mathbb{W}}$, and $a_0 = \det\hat{\mathbb{W}}$ for every $N \times N$ matrix (here we have $N = 3$).

(d) 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 $\bar{\omega} = \omega^T_L + \omega^L_R + \omega^R_T$ over the contribution to the observable added up for the transitions around the cycle $T \to L \to R \to T$.
The result in (c) is written in a form where this is trivial.

(e) Verify that $a_0(s)|_{s=0} = 0$. Why should that be true for every transition matrix?
The result in (c) is written in a form where this is trivial. It is true in general because for $s = 0$ we recover the transition matrix $\mathbb{W}$, which has an eigenvalue zero.

(bonus) 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? For the general case with N states we have

$$0 = P(\lambda(s); s) = \sum_{j=0}^{N} a_j(s)\, \lambda^j(s)$$

such that the implicit function theorem provides

$$0 = \frac{\mathrm{d}}{\mathrm{d}s} P(\lambda(s); s) = \sum_{j=1}^{N} a_j(s)\, j\, \lambda^{j-1}(s)\, \frac{\mathrm{d}\lambda(s)}{\mathrm{d}s} + \sum_{j=0}^{N} \frac{\mathrm{d}a_j(s)}{\mathrm{d}s}\, \lambda^j(s)$$

All terms that contain non-vanishing powers of $\lambda(s)$ vanish for $s = 0$ because $\lambda(s = 0) = 0$. Therefore, for $J = \mathrm{d}\lambda(s)/\mathrm{d}s|_{s=0}$ we find

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

which implies the states relation.

(f) Determine the current J for the present example.

$$J = \frac{ud}{(u + 2d)\,(u + r + l)}\,(r - l)\,\bar{\omega}$$

How does it differ for different observables ω?
The currents for different observables only differ by different values of the factor $\bar{\omega}$. This is due to the fact that the Markov process only has a single cycle.