MATH858D

MARKOV CHAINS

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Contents

1. Discrete-time Markov chains

Think about the following problem.

> **Example 1 (Gambler's ruin).** Imagine a gambler who has \$1 initially. At each discrete moment of time $t = 0, 1, \ldots$, the gambler can play \$1 if he has it and win one more \$1 with probability p or lose it with probability $q = 1 - p$. If the gambler runs out of money, he is ruined and cannot play anymore. What is the probability that the gambler will be ruined?

The gambling process described in this problem exemplifies a discrete-time Markov chain. In general, a discrete-time Markov chain is defined as a sequence of random variables $(X_n)_{n\geq 0}$ taking a finite or countable set of values and characterized by the Markov property: the probability distribution of X_{n+1} depends only of the probability distribution of X_n and does not depend on X_k for all $k \leq n-1$. We will denote the this discrete set of values by S and call it *the set of states*.

Definition 1. *We say that a sequence of random variables $(X_n)_{n\geq 0}$, where*

$$X_n : \Omega \to S \subset \mathbb{Z},$$

is a Markov chain with initial distribution λ and transition matrix $P = (p_{ij})_{i,j\in S}$ if

1. *X_0 has distribution $\lambda = \{\lambda_i \mid i \in S\}$ and*
2. *the Markov property holds:*

$$\mathbb{P}(X_{n+1} = i_{n+1} \mid X_n = i_n, \ldots, X_0 = i_0) = \mathbb{P}(X_{n+1} = i_{n+1} \mid X_n = i_n) = p_{i_n i_{n+1}}.$$

We will denote the Markov chain by $\mathsf{Markov}(P, \lambda)$. Note that the ith row of P is the probability distribution for X_{n+1} conditioned on the fact that $X_n = i$. Therefore, all entries of the matrix P are nonnegative, and the row sums are equal to one:

$$p_{ij} \geq 0, \quad \sum_{j\in S} \mathbb{P}(X_{n+1} = j \mid X_n = i) = \sum_{j\in S} p_{ij} = 1.$$

A matrix P satisfying these conditions in called *stochastic*.

Some natural questions about a Markov chain are:

- What is the equilibrium probability distribution, i.e., the one that is preserved from step to step?
- Does the probability distribution of X_n tend to the equilibrium distribution?
- How one can find the probability to reach some particular subset of states $A \subset S$? What is the expected time to reach this subset of states?

- Suppose we have selected two disjoint subsets of states A and B. What is the probability to reach first B rather than A starting from a given state? What is the expected time to reach B starting from A?

Prior to addressing these question, we will go over some basic concepts.

1.1. **Time evolution of the probability distribution.** If the set of states S is finite, i.e., if $|S| = N$, then P^n is merely the nth power of P. If S is infinite, we define P^n by

$$(P^n)_{ij} \equiv p_{ij}^{(n)} = \sum_{i_1 \in S} \cdots \sum_{i_{n-1} \in S} p_{ii_1} p_{i_1 i_2} \cdots p_{i_{n-1} j}.$$

Notation $\mathbb{P}_i(X_n = j)$ denotes the probability that the Markov process starting at i at time 0 will reach state j at time n:

$$\mathbb{P}_i(X_n = j) := \mathbb{P}(X_n = j \mid X_0 = i).$$

Theorem 1. *Let $(X_n)_{n \geq 0}$ be a Markov chain with initial distribution λ and transition matrix P. Then for all $n, m \geq 0$*

(1) $\mathbb{P}(X_n = j) = (\lambda P^n)_j$;
(2) $\mathbb{P}_i(X_n = j) = \mathbb{P}(X_{n+m} = j \mid X_m = i) = p_{ij}^{(n)}$.

Proof. (1)

$$\begin{aligned}
\mathbb{P}(X_n = j) &= \sum_{i_0 \in S} \cdots \sum_{i_{n-1} \in S} \mathbb{P}(X_n = j, X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) \\
&= \sum_{i_0 \in S} \cdots \sum_{i_{n-1} \in S} \mathbb{P}(X_n = j \mid X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) \mathbb{P}(X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) \\
&= \sum_{i_0 \in S} \cdots \sum_{i_{n-1} \in S} \mathbb{P}(X_n = j \mid X_{n-1} = i_{n-1}) \mathbb{P}(X_{n-1} = i_{n-1} \mid X_{n-2} = i_{n-1}) \ldots \mathbb{P}(X_0 = i_0) \\
&= \sum_{i_0 \in S} \cdots \sum_{i_{n-1} \in S} \lambda_{i_0} p_{i_0 i_1} \ldots p_{i_{n-1} j} = (\lambda P^n)_j.
\end{aligned}$$

(2) The second statement is proven similarly.

□

1.2. **Communicating classes and irreducibility.** We say that state i *leads to* state j (denote it by $i \longrightarrow j$) if

$$\mathbb{P}_i(X_n = j \text{ for some } n \geq 0) > 0.$$

If i leads to j and j leads to i we say that i and j *communicate* and write $i \longleftrightarrow j$. Note that i leads to j if and only if one can find a finite sequence $i_1, \ldots, i_{n-1}$ such that

$$p_{ii_1} > 0,\ p_{i_1 i_2} > 0,\ \ldots,\ p_{i_{n-1} j} > 0.$$

This, in turn, is equivalent to the condition that $p_{ij}^{(n)} > 0$ for some n.

The relation $\longleftrightarrow$ is an equivalence relation as it is

(1) symmetric as if $i \longleftrightarrow j$ then $j \longleftrightarrow i$;

(2) reflective, i.e., $i \longleftrightarrow i$;
(3) transitive, as $i \longleftrightarrow j$ and $j \longleftrightarrow k$ imply $i \longleftrightarrow k$.

Therefore, the set of states is divided into equivalence classes with respect to the relation $\longleftrightarrow$ called *communicating classes*.

Definition 2. *We say that a communicating class C is closed if*

$$i \in C, i \longrightarrow j \text{ imply } j \in C.$$

Once the chain jumps into a closed class, it stays there forever.

A state i is called *absorbing* if $\{i\}$ is a closed class. In the corresponding network, the vertex i has either only incoming edges, or no incident edges at all.

Example 2 Let us identify the states in the Gambler's ruin Markov chain 1 with the number of dollars at each of them. It is easy to see that states $\{1, 2, \ldots\} =: C_1$ constitute a communication class. The class C_1 is not closed because state $1 \in C_1$ leads to state $0 \notin C_1$. State 0 is a closed communicating class $\{0\} =: C_0$ and an absorbing state.

Definition 3. *A Markov chain whose set of states S is a single communicating class is called irreducible.*

Example 3 Let us consider a set of 7 identical particles shaped like balls interacting according to a sticky potential. I.e., the particles do not interact, when they do not touch each other, and they stick together as they touch forming a bond. Some amount of energy needs to be spent in order to break a bond. One example of such a system is a toy constructor consisting of magnetic sticks and steel balls. Another example is micron-size styrofoam balls immersed in water. M. Brenner's and V. Manoharan's group (Harvard University) conducted a number of physical experiments with such balls. M. Holmes-Cerfon and collaborators developed an efficient numerical algorithm for enumeration all possible configurations of particles and calculating transition rates between the configurations. A complete enumeration has been done for up to 14 particles, an a partial one for up to 19 [13]. One can model the dynamics of such a particle system as a continuous-time Markov chain which, in turn, can be converted into a jump chain, i.e., a discrete-time Markov chain. Such a jump chain for 7 particles is displayed in Fig. 1. The numbers next to the arrows are the transition probabilities. This chain was obtained from Fig. 6 in [12]. This Markov chain is **irreducible** because the process starting at any configuration, can reach any other configuration. While there are no direct jumps between states 2 and 4, the transitions between them can happen in two jumps. So is true for states 1 and 5. The transition matrix for this chain is given by:

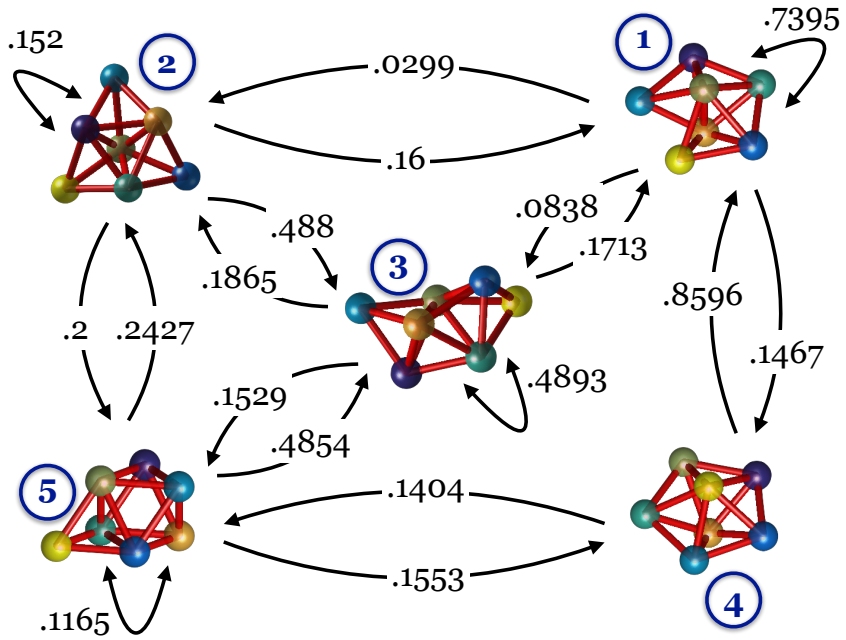


FIGURE 1. A jump chain for 7 particles interacting according to a sticky potential obtained from Fig. 6 in [12].

$$P = \begin{bmatrix} 0.7395 & 0.0299 & 0.0838 & 0.1467 & 0 \\ 0.1600 & 0.1520 & 0.4880 & 0 & 0.2000 \\ 0.1713 & 0.1865 & 0.4893 & 0 & 0.1529 \\ 0.8596 & 0 & 0 & 0 & 0.1404 \\ 0 & 0.2427 & 0.4854 & 0.1553 & 0.1165 \end{bmatrix} \tag{1}$$

1.3. **Hitting times and absorption probabilities.**

Definition 4. *Let $(X_n)_{n\geq 0}$ be a Markov chain with transition matrix P. The hitting time of a subset $A \subset S$ is the random variable $\tau_A : \Omega \to \{0, 1, 2, \ldots\} \cup \{\infty\}$ given by*

$$\tau^A = \inf\{n \geq 0 \mid X_n \in A\},$$

where we agree that $\inf \emptyset = \infty$.

Definition 5.

- *The probability that $(X_n)_{n\geq 0}$ ever hits A starting from state i is*

$$h_i^A = \mathbb{P}_i(\tau^A < \infty). \tag{2}$$

- *If A is a closed class, h_i^A is called the absorption probability.*

- *The mean time taken for $(X_n)_{n\geq 0}$ to reach A starting from i is*

$$k_i^A = E_i[\tau^A] \equiv E[\tau^A | X_0 = i] = \sum_{n<\infty} n\mathbb{P}_i(\tau^A = n) + \infty \mathbb{P}_i(\tau^A = \infty). \tag{3}$$

Example 4 In the Gambler's ruin example 1, a good question to ask is what is the probability that the gambler will eventually run out of money if initially he has i dollars. If $p \leq 1/2$, this probability is 1. The next question is what is the expected time for the gambler to run out of money. Using the just introduced notations, one needs to find $h_i^{\{0\}}$ and, if $h_i^{\{0\}} = 1$, what is $k_i^{\{0\}}$.

The quantities h_i^A and k_i^A can be calculated by solving certain linear equations.

Theorem 2. *The vector of hitting probabilities $h^A = \{h_i^A \mid i \in S\}$ is the minimal nonnegative solution to the system of linear equations*

$$\begin{cases} h_i^A = 1, & i \in A \\ h_i^A = \sum_{j\in S} p_{ij} h_j^A, & i \notin A. \end{cases} \tag{4}$$

(Minimality means that if $x = \{x_i \mid i \in S\}$ is another solution with $x_i \geq 0$ for all i, then $h_i^A \leq x_i$ for all i.)

Proof. First we show that the hitting probabilities satisfy Eq. (4). Indeed, if $i \in A$ then $\tau^A = 0$ and hence $\mathbb{P}_i(\tau^A < \infty) = 1$. If $i \notin A$, then

$$\begin{aligned} \mathbb{P}_i(\tau^A < \infty) &= \sum_{j\in S} \mathbb{P}_i(\tau^A < \infty \mid X_1 = j)\mathbb{P}_i(X_1 = j) \\ &= \sum_{j\in S} \mathbb{P}_j(\tau^A < \infty) p_{ij} = \sum_{j\in S} h_j^A p_{ij}. \end{aligned}$$

Now we show that if $x = \{x_i \mid i \in S\}$ is another nonnegative solution of Eq. (4) then $x_i \geq h_i^A$ for all $i \in S$. If $i \in A$ then $h_i^A = x_i = 1$. If $i \notin A$, we have

$$\begin{aligned} x_i =& \sum_{j\in S} p_{ij} x_j = \sum_{j\in A} p_{ij} + \sum_{j\notin A} p_{ij} x_j = \sum_{j\in A} p_{ij} + \sum_{j\notin A} p_{ij} \sum_{k\in S} p_{jk} x_k \\ =& \sum_{j\in A} p_{ij} + \sum_{j\notin A} p_{ij} \left(\sum_{k\in A} p_{jk} + \sum_{k\notin A} p_{jk} x_k \right) \\ =& \mathbb{P}_i(\tau^A = 1) + \mathbb{P}_i(\tau^A = 2) + \sum_{j\notin A} \sum_{k\notin A} p_{ij} p_{jk} x_k. \end{aligned}$$

Continuing in this manner we obtain

$$\begin{aligned} x_i =& \sum_{k=1}^{n} \mathbb{P}_i(\tau^A = k) + \sum_{j_1 \notin A} \cdots \sum_{j_n \notin A} p_{ij_1} p_{j_1 j_2} \cdots p_{j_{n-1} j_n} x_{j_n} \\ =& \mathbb{P}_i(\tau^A \leq n) + \sum_{j_1 \notin A} \cdots \sum_{j_n \notin A} p_{ij_1} p_{j_1 j_2} \cdots p_{j_{n-1} j_n} x_{j_n}. \end{aligned}$$

Since $x_j \geq 0$ for all $j \in S$, the last term in the last sum is nonnegative. Therefore,

$$x_i \geq \mathbb{P}_i(\tau^A \leq n) \quad \text{for} \quad \text{all} \quad n.$$

Hence

$$x_i \geq \lim_{n \to \infty} \mathbb{P}_i(\tau^A \leq n) = \mathbb{P}_i(\tau^A < \infty) = h_i.$$

□

Theorem 3. *The vector of mean hitting times $k^A = \{k_i^A \mid i \in S\}$ is the minimal nonnegative solution to the system of linear equations*

$$\begin{cases} k_i^A = 0, & i \in A \\ k_i^A = 1 + \sum_{j \in S} p_{ij} k_j^A, & i \notin A. \end{cases} \tag{5}$$

Proof. First we show that the mean hitting times satisfy Eq. (5). Indeed, if $i \in A$ the $k_i^A = 0$ as $\tau^A = 0$. Let us consider two cases.
Case 1: there is $i^* \in S \backslash A$ such that $h_{i^*}^A < 1$.
Case 2: for all $i \in S \backslash A$ such that $h_i^A = 1$.
In Case 1, Eq. (4) implies that all $h_i^A < 1$ for $i \notin A$ such that $i \longrightarrow i^*$. In this case, all $k_i^A = \infty$ such that $i \longrightarrow i^*$ by Eq. (3). Hence Eq. (5) holds. Let us consider Case 2. If $i \notin A$ then

$$\begin{aligned} k_i^A =& E_i[\tau^A] = \sum_{n=1}^{\infty} n \mathbb{P}(\tau^A = n \mid X_0 = i) \\ =& \sum_{n=1}^{\infty} n \sum_{j \in S} \mathbb{P}(\tau^A = n \mid X_1 = j,\ X_0 = i) \mathbb{P}_i(X_1 = j) \end{aligned}$$

We can switch order of summation because all terms are positive (this follows from the monotone convergence theorem). Also the Markov property implies that

$$\mathbb{P}(\tau^A = n \mid X_1 = j,\ X_0 = i) = \mathbb{P}(\tau^A = n \mid X_1 = j).$$

We continue:

$$\begin{aligned}
k_i^A =& \sum_{j\in S}\sum_{n=1}^{\infty} n\mathbb{P}(\tau^A = n \mid X_1 = j)\mathbb{P}_i(X_1 = j)\\
=& \sum_{j\in S}\left(\sum_{m=0}^{\infty}(m+1)\mathbb{P}(\tau^A = m \mid X_0 = j)p_{ij}\right)\\
=& \sum_{j\in S}\left(\sum_{m=0}^{\infty} m\mathbb{P}(\tau^A = m \mid X_0 = j)p_{ij} + \sum_{m=0}^{\infty}\mathbb{P}(\tau^A = m \mid X_0 = j)p_{ij}\right)\\
=& \sum_{j\in S} p_{ij}k_j^A + \sum_{j\in S} p_{ij}\sum_{m=0}^{\infty}\mathbb{P}(\tau^A = m \mid X_0 = j).
\end{aligned}$$

Now we use the observe that

$$\sum_{m=0}^{\infty}\mathbb{P}(\tau^A = m \mid X_0 = j) = h_j^A = 1$$

since we are considering Case 2. Finally,

$$\sum_{j\in S} p_{ij} = 1$$

as this is a row sum of the transition matrix. As a result, we obtain what we have desired:

$$k_i^A = 1 + \sum_{j\in S} p_{ij}k_j^A.$$

Now we show that if $\{y_i \mid i \in S\}$ with $y_i \geq 0$ for every $i \in S$ is another solution of Eq. (5) then $k_i^A \leq y_i$ for all $i \in S$. If $i \in A$, then $k_i^A = y_i = 0$. For $i \notin A$ we have:

$$\begin{aligned}
y_i =& 1 + \sum_{j\in S} p_{ij}y_j = 1 + \sum_{j\notin A} p_{ij}y_j = 1 + \sum_{j\notin A} p_{ij}\left(1 + \sum_{k\notin A} p_{jk}y_k\right)\\
=& \mathbb{P}_i(\tau^A \geq 1) + \mathbb{P}_i(\tau^A \geq 2) + \sum_{j\notin A}\sum_{k\notin A} p_{ij}p_{jk}y_k.
\end{aligned}$$

Continuing in this manner we obtain:

$$\begin{aligned}
y_i =& \mathbb{P}_i(\tau^A \geq 1) + \mathbb{P}_i(\tau^A \geq 2) + \ldots \mathbb{P}_i(\tau^A \geq n) + \sum_{j_1\notin A}\ldots\sum_{j_n\notin A} p_{ij_1}p_{j_1j_2}\ldots p_{j_{n-1}j_n}y_{j_n}\\
=& \mathbb{P}_i(\tau^A) = 1 + 2\mathbb{P}_i(\tau^A = 2) + \ldots + n\mathbb{P}_i(\tau^A \geq n) + \sum_{j_1\notin A}\ldots\sum_{j_n\notin A} p_{ij_1}p_{j_1j_2}\ldots p_{j_{n-1}j_n}y_{j_n}.
\end{aligned}$$

Since $y_i \geq 0$, so is the last term. Hence

$$y_i \geq \mathbb{P}_i(\tau^A = 1) + 2\mathbb{P}_i(\tau^A = 2) + \ldots n\mathbb{P}_i(\tau^A \geq n) \text{ for all } n.$$

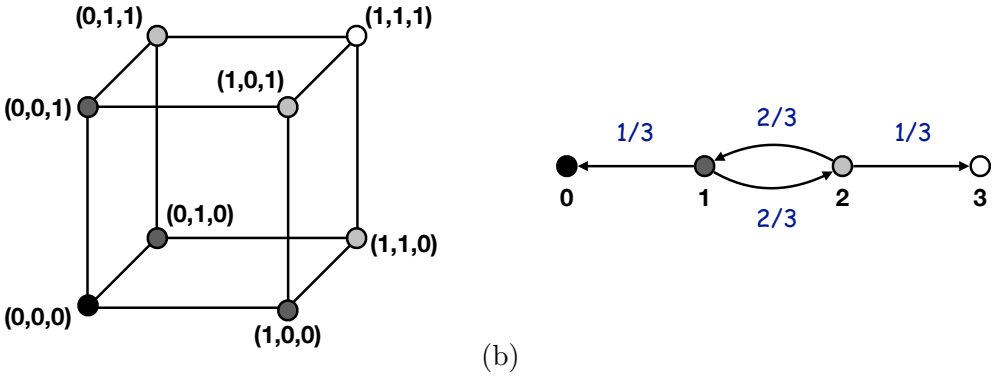
Therefore,

$$y_i \geq \sum_{n=1}^{\infty} n\mathbb{P}_i(\tau_i = n) = E_i[\tau^A] = k_i^A.$$

□

Example 5 Consider a particle wandering along the edges of a cube Fig. 2(a). If the particle reaches vertices $(0,0,0)$ and $(1,1,1)$, it disappears. From each of the other vertices (colored with a shade of grey in Fig. 2(a)), it moves to any vertex connected to it via an edge with equal probabilities. Suppose that the particle is initially located at the vertex $(0,0,1)$. Find the probability that it will disappear at vertex $(0,0,0)$.
Hint: consider four subsets of vertices:
$0 \equiv \{(0,0,0)\}$,
$1 \equiv \{(1,0,0),(0,1,0),(0,0,1)\}$,
$2 \equiv \{(0,1,1),(1,0,1),(0,1,1)\}$, *and*
$3 \equiv \{(1,1,1)\}$
as shown in the Fig. 2(b). Find the probabilities to jump along each arrow in Fig. 2(b). Denote by P_i the probability for the particle to disappear at vertex $(0,0,0)$ starting from subset i, $i = 0,1,2,3$. Write an appropriate system of equations for P_i and solve it.

Solution 1: Transition probabilities between the subsets 0, 1, 2 and 3 are



(a) (b)

FIGURE 2. Illustration for Example 5

shown in Fig. 2(b). Let P_i be the probability for the particle to disappear at $(0,0,0)$ provided that it is initially at the subset of vertices i. Then we

have:

$$\begin{aligned} P_0 &= 1; \\ P_1 &= \frac{1}{3}P_0 + \frac{2}{3}P_2; \\ P_2 &= \frac{2}{3}P_1 + \frac{1}{3}P_3; \\ P_3 &= 0. \end{aligned}$$

The solution of this system is $P_0 = 1$, $P_1 = \frac{3}{5}$, $P_2 = \frac{2}{5}$, $P_3 = 0$.

Solution 2: Transition probabilities between the subsets 0, 1, 2 and 3 are shown in Fig. 2(b). The probability to get to 0 starting from 1 is the sum of probabilities to get to 0 from nth visit of 1:

$$P_1 = \sum_{n=1}^{\infty} \frac{1}{3}\left(\frac{2}{3}\right)^{2(n-1)} = \frac{1}{3}\frac{1}{1-\frac{4}{9}} = \frac{3}{5}.$$

Answer: $\frac{3}{5}$.

Example 6 Consider a particle wandering along the edges of a cube like in Example 5 except for now the only absorbing state is the vertex $(0,0,0)$. If particle is at any other vertex, it goes to one of the vertices connected to it by an edge with equal probability. Find the expected time for a process starting at each vertex to be absorbed at $(0,0,0)$.

Solution: Taking symmetry into account, we define a reduced Markov

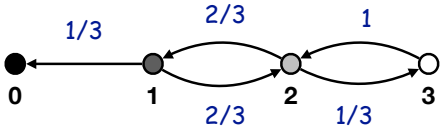


FIGURE 3. Illustration for Example 6

chain shown in Fig. 3. Let $k_i = \mathbb{E}_i[\tau^0]$ be the expected first passage time to $(0,0,0)$ provided that it is initially at the subset of vertices i. Then we have:

$$\begin{aligned} k_0 &= 0; \\ k_1 &= 1 + \frac{1}{3}k_0 + \frac{2}{3}k_2; \\ k_2 &= 1 + \frac{2}{3}k_1 + \frac{1}{3}k_3; \\ k_3 &= 1 + k_2. \end{aligned}$$

The solution of this system is $k_0 = 0$, $k_1 = 7$, $k_2 = 9$, $k_3 = 10$.

1.4. **Solving recurrence relationships.** In the case where the Markov chain has an infinite set of states, $\mathbb{Z}$ or $\{0, 1, 2, \ldots\}$, and only transitions between nearest neighbors are possible, Eqs. (4) and (5) become linear 2nd order recurrence relationships, homogeneous and nonhomogeneous respectively. A recipe for solving linear recurrence relationships with constant coefficients, homogeneous and nonhomogeneous, can be found e.g. here (a presentation by Niloufar Shafiei).

Second order recurrence relationships can be solved uniquely if one has two initial (boundary) conditions. However, if the set of states $S = \{0, 1, 2, \ldots\}$ and $A = \{0\}$ (as in the Markov chain Gambler's ruin 1), Eqs. (4) and (5) have only one boundary condition. The solutions h^A and k^A are determined by the additional requirements that they must be minimal and nonnegative.

Now we consider the "birth-and-death" Markov chain where the coefficients are of the transition matrix P are

$$P_{00} = 1,\ P_{i,i+1} = p_i,\ P_{i,i-1} = q_i,\ p_i + q_i = 1,\ i \geq 1.$$

In this chain, 0 is an absorbing state, and we wish to calculate the absorption probability starting from an arbitrary state i. Eq. (4) gives:

$$h_0 = 1, \quad h_i = q_i h_{i-1} + p_i h_{i+1}, \quad i \geq 1.$$

This recurrence relationship cannot be solved by the tools for the case of constant coefficients. However, another technique works in this case. Consider

$$u_i := h_{i-1} - h_i.$$

Subtracting h_i from both parts of $h_i = q_i h_{i-1} + p_i h_{i+1}$ and taking into account that $q_i + p_i = 1$ we get:

$$p_i u_{i+1} = q_i u_i.$$

Therefore,

$$u_{i+1} = \left(\frac{q_i}{p_i}\right) u_i = \left(\frac{q_i q_{i-1} \ldots q_1}{p_i p_{i-1} \ldots p_1}\right) u_1 =: \gamma_i u_1.$$

Then

$$u_1 + u_2 + \ldots + u_i = h_0 - h_1 + h_1 - h_2 + \ldots + h_{i-1} - h_i = h_0 - h_i.$$

Hence

$$h_i = h_0 - u_1(1 + \gamma_1 + \ldots + \gamma_{i-1}) = 1 - u_1 \sum_{j=0}^{i-1} \gamma_j,$$

as $h_0 = 1$. Here we have defined $\gamma_0 = 1$. Note that u_1 cannot be determined from the boundary condition $h_0 = 1$. It has to be determined from the condition that h is the minimal nonnegative solution. Therefore, we need to consider two cases.

$\sum_{j=0}^{\infty} \gamma_j = \infty$**:** In this case, u_1 must be 0. Hence $h_i = 1$ for all $i \geq 0$. Hence the absorption probability is 1 for every i.

$\sum_{j=0}^{\infty}\gamma_j < \infty$**:** In this case, the minimal nonnegative solution will be the one where

$$h_i \to 0 \quad \text{as} \quad i \to \infty.$$

This will take place if we set

$$u_1 = \left(\sum_{j=0}^{\infty}\gamma_j\right)^{-1}.$$

Then

$$h_i = 1 - \frac{\sum_{j=0}^{i-1}\gamma_j}{\sum_{j=0}^{\infty}\gamma_j} = \frac{\sum_{j=i}^{\infty}\gamma_j}{\sum_{j=0}^{\infty}\gamma_j}.$$

Therefore, the absorption probabilities $h_i < 1$ for $i \geq 1$.

Example 7 A gambler has \$1 initially. At each round, he either wins \$1 with probability p or loses \$1 with probability $q = 1 - p$ playing agains an infinitely rich casino. Find the probability that he gets broke, i.e., his capital is down to \$0.
Solution: Let P_i be the probability to get to the situation of having \$0 provided that the initial amount is $\$i$. We have:

$$P_0 = 1;$$
$$P_i = pP_{i+1} + qP_{i-1},\ 1 \leq i < \infty.$$

Observe that the probability to get to \$0 starting from \$1 is the same as the one to get to \$1 starting from \$2. Therefore, the probability to get to \$0 starting from \$2 is the product of the probabilities to get to \$1 from \$2 and to get to \$0 from \$1, i.e., $P_2 = P_1^2$. Hence, we get the following quadratic equation for P_1, taking into account that $P_0 = 1$ and $q = 1 - p$:

$$P_1 = pP_1^2 + 1 - p.$$

Solving it, we get two roots: 1 and $\frac{1-p}{p}$. If $p \leq 1/2$, then $\frac{1-p}{p} \geq 1$, hence the only suitable solution is $P_1 = 1$. If $p > 1/2$, then $\frac{1-p}{p} < 1$, and we should pick the root $P_1 = \frac{1-p}{p}$. One can see it as follows. Suppose that there is a maximal amount of money $\$N$ that the gambler can get from the casino. Performing a calculation similar to the one in the previous problem and letting $N \to \infty$, one can get that $P_1 \to q/p = (1-p)/p$ as $N \to \infty$.
Answer: $P_1 = 1$ if $p \leq 1/2$, and $P_1 = \frac{1-p}{p}$ if $p > 1/2$.

1.5. **Recurrence and transience.**

Definition 6. *Let $(X_n)_{n\geq 0}$ be a Markov chain with transition matrix P. We say that a state i is recurrent if*

$$\mathbb{P}_i(X_n = i \text{ for infinitely many } n) = 1. \tag{6}$$

We say that a state i is transient if

$$\mathbb{P}_i(X_n = i \text{ for infinitely many } n) = 0. \tag{7}$$

Surprisingly at the first glance, one can show that every state is either recurrent or transient. This is the consequence of the Markov property. To prove this, we will need the following definitions.

Definition 7.

- *The first passage time to state i is the random variable T_i defined by*
$$T_i(\omega) = \inf\{n \geq 1 \mid X_n(\omega) = i\}, \quad \text{where} \quad \inf \emptyset = \infty.$$
- *The rth passage time to state i is the random variable $T_i^{(r)}$ defined inductively by*
$$T_i^{(0)} = 0, \quad T_i^{(r+1)} = \inf\{n \geq T_i^{(r)} + 1 \mid X_n(\omega) = i\}, \quad r = 0, 1, 2, \ldots.$$
- *The length of rth excursion to i is*
$$S_i^{(r)} = \begin{cases} T_i^{(r)} - T_i^{(r-1)} & \text{if } T_i^{(r-1)} < \infty \\ 0 & \text{otherwise.} \end{cases}$$
- *The return probability is defined by*
$$f_i = \mathbb{P}_i(T_i < \infty).$$
- *The number of visits V_i of state i is the random variable that can be written as the sum of indicator functions*
$$V_i = \sum_{n=0}^{\infty} 1_{\{X_n = i\}}.$$

Note that

$$\begin{aligned} E_i[V_i] =& E_i\left[\sum_{n=0}^{\infty} 1_{\{X_n=i\}}\right] = \sum_{n=0}^{\infty} E\left[1_{\{X_n=i\}} | X_0 = i\right] \\ =& \sum_{n=0}^{\infty} \mathbb{P}_i(X_n = i) = \sum_{n=0}^{\infty} p_{ii}^{(n)}. \end{aligned} \tag{8}$$

Also note that the conditions for a state to be recurrent or transient can be written as

- state i is recurrent if $\mathbb{P}_i(V_i = \infty) = 1$;
- state i is transient if $\mathbb{P}_i(V_i = \infty) = 0$.

Theorem 4. *The following dichotomy holds:*

(1) *if $\mathbb{P}_i(T_i < \infty) = 1$, then i is recurrent and $\sum_{n=0}^{\infty} p_{ii}^{(n)} = \infty$;*

(2) *if* $\mathbb{P}_i(T_i < \infty) < 1$, *then* i *is transient and* $\sum_{n=0}^{\infty} p_{ii}^{(n)} < \infty$.

In particular, every state is either transient or recurrent.

Proof. (1) Let us denote $\mathbb{P}_i(T_i < \infty)$ by f_i. First show that

$$\mathbb{P}_i(V_i > r) = f_i^r.$$

$$\begin{aligned}\mathbb{P}_i(V_i > r) =& \mathbb{P}_i(T_i^{(r)} < \infty) = \mathbb{P}_i(S_i^{(r)} < \infty \mid T_i^{(r-1)} < \infty)\mathbb{P}_i(T_i^{(r-1)} < \infty)\\ =& \mathbb{P}_i(S_i^{(r)} < \infty \mid T_i^{(r-1)} < \infty)\mathbb{P}_i(S_i^{(r-1)} < \infty \mid T_i^{(r-2)} < \infty)\dots\mathbb{P}_i(T_i < \infty)\\ =& f_i^r.\end{aligned}$$

(2) If $f_i = \mathbb{P}_i(T_i < \infty) = 1$, then

$$\mathbb{P}_i(V_i = \infty) = \lim_{r\to\infty} \mathbb{P}_i(V_i > r) = \lim_{r\to\infty} f_i^r = \lim_{r\to\infty} 1 = 1.$$

Hence i is recurrent and $\sum_{n=0}^{\infty} p_{ii}^{(n)} = E_i[V_i] = \infty$.

(3) If $f_i = \mathbb{P}_i(T_i < \infty) < 1$, then

$$\mathbb{P}_i(V_i = \infty) = \lim_{r\to\infty} \mathbb{P}_i(V_i > r) = \lim_{r\to\infty} f_i^r = 0.$$

Hence i is transient and

$$\sum_{n=0}^{\infty} p_{ii}^{(n)} = E_i[V_i] = \sum_{r=0}^{\infty} \mathbb{P}_i(V_i > r) = \sum_{r=0}^{\infty} f_i^r = \frac{1}{1-f_i} < \infty.$$

□

Now I will list some facts about recurrence and transience. I will not prove them. Proofs can be found e.g. in [1].

- In a communicating class, states are either all transient or all recurrent.
- Every recurrent class is closed.
- Every finite closed class is recurrent.
- For a simple random walk on $\mathbb{Z}$, where the entries of the transition matrix are all zeros except for $p_{i,i+1} = q$, $p_{i,i-1} = 1 - q$, all states are transient if $q \neq 1/2$, and all states are recurrent if $q = 1/2$.
- For a simple symmetric random walk on $\mathbb{Z}^2$, all states are recurrent.
- For a simple symmetric random walk on $\mathbb{Z}^n$, $n \geq 3$, all states are transient.

1.6. **Invariant distributions and measures.**

Definition 8. *A measure on a Markov chain is any vector* $\lambda = \{\lambda_i \geq 0 \mid i \in S\}$. *A measure is invariant (a. k. a stationary or equilibrium) if*

$$\lambda = \lambda P.$$

A measure is a distribution if, in addition, $\sum_{i\in S} \lambda_i = 1$.

Theorem 5. *Let the set of states S of a Markov chain $(X_n)_{n\geq 0}$ be finite. Suppose that for some $i \in S$*

$$\mathbb{P}_i(X_n = j) = p_{ij}^{(n)} \to \pi_j \text{ as } n \to \infty \text{ for all } j \in S.$$

Then $\pi = \{\pi_j \mid j \in S\}$ is an invariant distribution.

Proof. Since $p_{ij}^{(n)} \geq 0$ we have $\pi_j \geq 0$. Show that $\sum_{j\in S} \pi_j = 1$. Since S is finite, we can swap the order of taking limit and summation:

$$\sum_{j\in S} \pi_j = \sum_{i\in S} \lim_{n\to\infty} p_{ij}^{(n)} = \lim_{n\to\infty} \sum_{i\in S} p_{ij}^{(n)} = 1.$$

Show that $\pi = \pi P$:

$$\pi_j = \lim_{n\to\infty} p_{ij}^{(n)} = \lim_{n\to\infty} \sum_{k\in S} p_{ik}^{(n-1)} p_{kj} = \sum_{k\in S} \lim_{n\to\infty} p_{ik}^{(n-1)} p_{kj} = \sum_{k\in S} \pi_k p_{kj}.$$

□

Remark If the set of states is not finite, then the one cannot exchange summation and taking limit. For example, $\lim_{n\to\infty} p_{ij}^{(n)} = 0$ for all i, j for a simple symmetric random walk on $\mathbb{Z}$. $\{\pi_i = 0 \mid i \in \mathbb{Z}\}$ is certainly an invariant measure, but it is not a distribution.

The existence of an invariant distribution does not guarantee convergence to it. For example, consider the two-state Markov chain with transition matrix

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The distribution $\pi = (1/2, 1/2)$ is invariant as

$$(1/2, 1/2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (1/2, 1/2).$$

However, for any initial distribution $\lambda = (q, 1-q)$ where $q \in [0, 1/2) \cup (1/2, 1]$, the limit

$$\lim_{n\to\infty} P^n$$

does not exist as

$$P^{2k} = I, \quad P^{2k+1} = P.$$

In order to eliminate such cases, we introduce the concept of aperiodic states.

Definition 9. *Let us call a state i aperiodic, if $p_{ii}^{(n)} > 0$ for all sufficiently large n.*

Theorem 6. *Suppose P is irreducible and has an aperiodic state i. Then for all states j and k, $p_{jk}^{(n)} > 0$ for all sufficiently large n. In particular, all states are aperiodic.*

Proof. Since the chain is irreducible, there exist such r and s that $p_{ji}^{(r)} > 0$ and $p_{ik}^{(s)} > 0$. Then for sufficiently large n we have

$$p_{jk}^{(r+n+s)} = \sum_{i_1,\ldots,i_n\in S} p_{ji_1}^{(r)} p_{i_1 i_2} \cdots p_{i_{n-1} i_n} p_{i_n k}^{(s)} \geq p_{ji}^{(r)} p_{ii}^{(n)} p_{ik}^{(s)} > 0.$$

□

Definition 10. *We will call a Markov chain aperiodic if all its states are aperiodic.*

Theorem 7. *Suppose that $(X_n)_{n\geq 0}$ is a Markov chain with transition matrix P and initial distribution λ. Let P be irreducible and aperiodic, and suppose that P has an invariant distribution π. Then*

$$\mathbb{P}(X_n = j) \to \pi_j \text{ as } n \to \infty \text{ for all } j.$$

In particular,

$$p_{ij}^{(n)} \to \pi_j \text{ as } n \to \infty \text{ for all } i, j.$$

A proof of this theorem is found in [1]. In the case where the set of states is finite, this result can be proven by means of linear algebra. A building block of this proof is the Perron-Frobenius theorem.

Theorem 8. *Let A be an $N \times N$ matrix with nonnegative entries such that all entries of A^m are strictly positive for all $m > M$. Then*

1. *A has a positive eigenvalue $\lambda_0 > 0$ with corresponding left eigenvector x_0 where all entries are positive;*
2. *if $\lambda \neq \lambda_0$ is any other eigenvalue, then $|\lambda| < \lambda_0$.*
3. *λ_0 has geometric and algebraic multiplicity one.*

Let P be the stochastic matrix for a Markov chain with N states. For sufficiently large n, all entries of P^n for stochastic irreducible aperiodic matrices P become positive. The proof of this fact is similar to the one of Theorem 6. Furthermore, the largest eigenvalue of a stochastic matrix is equal to 1. Indeed, since the row sums of P are ones, $\lambda_0 = 1$ is an eigenvalue with the right eigenvector $e = [1, \ldots, 1]^\top$.

Now let us show that the other eigenvalues do not exceed $\lambda_0 = 1$ in absolute value. Let (λ, v) be an eigenvalue and a corresponding right eigenvector of a stochastic matrix P. We normalize v so that

$$v_i = \max_{k\in S} |v_k| = 1.$$

Since

$$\lambda v_i = \sum_{k\in S} p_{ik} v_k,$$

we have

$$|\lambda| = \left| \frac{1}{v_i} \sum_{k\in S} p_{ik} v_k \right| \leq \frac{1}{v_i} \sum_{k\in S} p_{ik} |v_k| \leq \sum_{k\in S} p_{ik} = 1.$$

Remark The fact that the eigenvalues of a stochastic matrix do not exceed 1 in absolute value is an instance of the Gershgorin Circle Theorem.

Theorem 9. *Every irreducible aperiodic Markov chain with a finite number of states N has a unique invariant distribution π. Moreover,*

$$\lim_{n\to\infty} qP^n = \pi \tag{9}$$

for any initial distribution q.

Proof. The Perron-Frobenius theorem applied to a finite stochastic irreducible aperiodic matrix P implies that the largest eigenvalue of P is $\lambda_0 = 1$ and all other eigenvalues are strictly less than 1 in absolute value. The left eigenvector π, corresponding to λ_0 has positive entries and can be normalized so that they sum up to 1. Hence,

$$\pi = \pi P, \quad \sum_{i=1}^{N} \pi_i = 1.$$

Now let us establish convergence. First we consider the case when P is diagonalizable:

$$P = V \Lambda U,$$

where Λ is the matrix with ordered eigenvalues along its diagonal:

$$\Lambda = \begin{pmatrix} 1 & & & \\ & \lambda_1 & & \\ & & \ddots & \\ & & & \lambda_{N-1} \end{pmatrix}, \quad 1 > |\lambda_1| \geq \ldots \geq |\lambda_{N-1}|,$$

V is the matrix of right eigenvectors of P: $PV = V\Lambda$, such that its first column is $e = [1, \ldots, 1]^\top$. $U = V^{-1}$ is the matrix of left eigenvectors of P: $UP = \Lambda U$. The first row of U is $\pi = [\pi_1, \ldots, \pi_N]$. One can check that if $UV = I_N$, these choices of the first column of V and the first row of U are consistent. Therefore, taking into account that $\sum_{i=1}^{N} q_i = 1$, we calculate:

$$\begin{aligned}
&\lim_{n\to\infty} qP^n \\
&= \lim_{n\to\infty} [q_1\ q_2\ \ldots\ q_N] \begin{pmatrix} 1 & * & * & * \\ 1 & * & * & * \\ & \ldots & & \\ 1 & * & * & * \end{pmatrix} \begin{pmatrix} 1 & & & \\ & \lambda_2^n & & \\ & & \ddots & \\ & & & \lambda_N^n \end{pmatrix} \begin{pmatrix} \pi_1 & \pi_2 & \ldots & \pi_N \\ * & * & * & * \\ & \ldots & & \\ * & * & * & * \end{pmatrix} \\
&= [1\ 0\ \ldots\ 0] \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{pmatrix} \begin{pmatrix} \pi_1 & \pi_2 & \ldots & \pi_N \\ * & * & * & * \\ & \ldots & & \\ * & * & * & * \end{pmatrix} \\
&= [\pi_1\ \pi_2\ \ldots\ \pi_N].
\end{aligned}$$

In the case when P is not diagonalizable, the argument is almost identical, just a bit more tedious. We consider the Jordan decomposition of P

$$P = VJU$$

where $U = V^{-1}$ and J is the Jordan form of of P, i.e., a block-diagonal matrix of the form:

$$J = \begin{bmatrix} 1 & & & \\ & J_1 & & \\ & & \ddots & \\ & & & J_r \end{bmatrix},$$

with the first block being 1×1 matrix $J_0 \equiv 1$, and respectively, the first column of V being $[1, \dots, 1]^\top$, and the first row of U being π – the right and left eigenvectors corresponding to the eigenvalue 1, and the other blocks J_i of sizes $m_i \times m_i$, where $1 \le m_i \le N-1$ and $m_1 + \ldots + m_r = N - 1$, of the form

$$J_i = \begin{bmatrix} \lambda_i & 1 & & \\ & \lambda_i & 1 & \\ & & \ddots & \ddots \\ & & & \lambda_i \end{bmatrix} =: \lambda_i I_{m_i \times m_i} + E. \tag{10}$$

Exercise (1) Check that the matrix E in Eq. (10) with ones right above the diagonal and all other entries zero is nilpotent. More precisely, $E^{m_i} = \mathbf{0}_{m_i \times m_i}$.

(2) Check that the matrices $\lambda_i I_{m_i \times m_i}$ and E commute.

(3) Check that

$$J_i^n = \sum_{k=0}^{m_i - 1} \begin{pmatrix} n \\ k \end{pmatrix} \lambda_i^{n-k} E^k.$$

(4) Argue that

$$\lim_{n \to \infty} J_i^n = \mathbf{0}_{m_i \times m_i}$$

provided that $|\lambda_i| < 1$.

(5) Now prove Eq. (9) for the case when P is not diagonalizable.

□

2. Time reversal and detailed balance

For Markov chains, the past and the future are independent given the present. This property is symmetric in time and suggests looking at Markov chains with time running backwards. On the other hand, convergence to equilibrium shows that the behavior is asymmetric in time. Hence, to complete the symmetry in time, we need to start with the equilibrium distribution.

For convenience, we will use the following notations:
$Markov(\lambda, P)$ denotes the discrete-time Markov chain with initial distribution λ and transition matrix P.
$Markov(\lambda, L)$ denotes a continuous-time Markov chain initial distribution λ and generator matrix L.

Theorem 10. *Let $(X_n)_{0\le n\le N}$ be $Markov(\pi, P)$, where P is irreducible and π is invariant. Define $Y_n = X_{N-n}$. Then $(Y_n)_{0\le n\le N}$ is $Markov(\pi, \hat{P})$ where the transition matrix $\hat{P} = (\hat{p}_{ij})$ defined by*

$$\pi_j p_{ji} = \pi_i \hat{p}_{ij} \text{ for all } i, j \in S.$$

Proof. Note that, since P is irreducible, all components of π are positive. We need to check the following three facts.

(1) Check that $\hat{P}$ is a stochastic matrix (i.e., all its entries are nonnegative and its row sums are equal to 1):

$$\hat{p}_{ij} = \frac{\pi_j}{\pi_i} p_{ji} \ge 0.$$

$$\sum_{j\in S} \hat{p}_{ij} = \frac{1}{\pi_i} \sum_{j\in S} \pi_j p_{ji} = \frac{\pi_i}{\pi_i} = 1.$$

In the last equation, we used the fact that π is invariant for P.

(2) Check that π is invariant for $\hat{P}$, i.e., that $\pi\hat{P} = \pi$:

$$\sum_{j\in S} \pi_j \hat{p}_{ji} = \sum_{j\in S} \pi_i p_{ij} = \pi_i \sum_{j\in S} p_{ij} = \pi_i \text{ for all } i \in S.$$

(3) Check that $(Y_n)_{0\le n\le N}$ satisfies Markov property.

$$\begin{aligned}&\mathbb{P}(Y_0 = i_0, Y_1 = i_1, \dots, Y_N = i_N) = \mathbb{P}(X_0 = i_N, X_1 = i_{N-1}, \dots, X_N = i_0)\\ =&\pi_{i_N} p_{i_N i_{N-1}} \cdots p_{i_1 i_0} = \hat{p}_{i_N i_{N-1}} \pi_{i_{N-1}} p_{i_{N-1} i_{N-2}} \cdots p_{i_1 i_0}\\ =&\dots = \hat{p}_{i_{N-1} i_N} \cdots \hat{p}_{i_0 i_1} \pi_{i_0}.\end{aligned}$$

Therefore, $(Y_n)_{0\le n\le N}$ satisfies Markov property.

□

Definition 11. *The chain $(Y_n)_{0\le n\le N}$ is called the time-reversal of $(X_n)_{0\le n\le N}$.*

Definition 12. *A stochastic matrix P and a measure λ are in detailed balance if*

$$\lambda_i p_{ij} = \lambda_j p_{ji}.$$

Suppose the set of states S is finite, the matrix P is irreducible, and the system is distributed according to the invariant distribution π. The condition of detailed balance means the following. Let $N_{i\to j}(n)$ be the number of transitions from i to j observed by time n. Then for all $i, j \in S$,

$$\lim_{n\to\infty} \frac{N_{i\to j}(n)}{N_{j\to i}(n)} = 1,$$

if P is in detailed balance with π. In words, over large intervals of times, on average, one observes equal numbers of transitions from i to j and from j to i for all $i, j \in S$ given the detailed balance.

The detailed balance condition gives us another way to check whether a given measure λ is invariant.

Theorem 11. *Let P and λ be in detailed balance. Then λ is invariant for P.*

Proof.

$$(\lambda P)_i = \sum_{j\in S} \lambda_j p_{ji} = \lambda_i \sum_{j\in S} p_{ij} = \lambda_i.$$

Hence $\lambda P = \lambda$. □

Definition 13. *Let $(X_n)_{n\geq 0}$ be $Markov(\lambda, P)$ where P is irreducible. We say that $(X_n)_{n\geq 0}$ is reversible if for all $N \geq 1$, $(X_{N-n})_{0\leq n\leq N}$ is $Markov(\lambda, P)$.*

Theorem 12. *Let P be an irreducible stochastic matrix and let λ be a distribution. Suppose that $(X_n)_{n\geq 0}$ is $Markov(\lambda, P)$. Then the following are equivalent:*

1. *$(X_n)_{n\geq 0}$ is reversible;*
2. *P and λ are in detailed balance.*

Proof. Both (1) and (2) imply that λ is invariant for P. Then both (1) and (2) are equivalent to the statement that $\hat{P} = P$. □

3. Markov Chain Monte Carlo methods

As we have discussed, Monte Carlo methods are those where random numbers are used in order to evaluate something nonrandom. Markov Chain Monte Carlo methods (MCMC) are those where the estimation is done via constructing a Markov Chain whose invariant distribution is the desired distribution. MCMC methods are used for numerical approximation of multidimensional integrals. Such integrals arise, e.g., in Bayesian parameter estimation, computational physics, and computational biology. For example, consider the problem of finding the expected value of $g(\eta)$ where η is a random variable with pdf $\pi(x)$, $x \in \mathbb{R}^d$:

$$E[g(\eta)] = \int_{x\in\mathbb{R}^d} g(x)\pi(x)dx. \tag{11}$$

Or, consider the problem of finding the expected value of $g(\eta)$ in the case where Ω is finite but huge, i.e., $|\Omega| = N$ where N is huge. Let $\pi(\omega)$ be the probability distribution on Ω, then

$$E[g(\eta)] = \sum_{\omega\in\Omega} g(\eta(\omega))\pi(\omega), \tag{12}$$

Note that in both of the cases, one rarely knows π per se. Instead, often only a measure f proportional to π is known. For example, think about the canonical pdf for n particles in 3D:

$$\mu(x,p) = \frac{1}{Z} e^{-\beta(V(x)+|p|^2/2)},\ Z = \int_{\mathbb{R}^{6n}} e^{-\beta(V(x)+|p|^2/2)} dxdp.$$

The normalization constant Z, except for some simple cases, cannot be evaluated analytically. Therefore, $\mu(x,p)$ is, strictly speaking, unknown. However, for each (x,p) one can calculate the measure

$$f(x,p) = e^{-\beta(V(x)+|p|^2/2)}$$

that is proportional to $\mu(x,p)$

Therefore, the problem is two-fold:

- The expected value is hard-to-evaluate due to either high dimensionality of the integral, so that numerical quadrature methods are unappreciable, or due to the huge number of summands in the sum (think about numbers like $N = 2^n$ where $n \sim 10^k$, $k = 2, 3, 4 \ldots$). Moreover, π is often far from being uniform, and some kind of importance sampling is necessary to be able to obtain a satisfactory estimate using a reasonable number of samples of η.
- The pdf or the probability distribution π is unknown. Instead, f, that is proportional to π, is given.

3.1. **Metropolis and Metropolis-Hastings algorithms.** We will explain the idea of the Metropolis algorithm on the example of the task of numerical approximation of the sum in Eq. (12) where Ω is a finite set, $|\Omega| = N$, N is huge. We wish to construct a discrete-time Markov chain $(X_n)_{n\geq 0}$, $X_n : \Omega \to \{1, \ldots, N\}$, i.e., where the each random variable X_n is simply an enumeration of the set of outcomes. Therefore, we may think that the set of states S and the set of outcomes Ω are identical. In order to be able to approximate the sum in Eq. (12), we need to design a transition matrix P so that the the desired measure f is invariant, and for any initial distribution λ, λP^n converges to $\pi := Z^{-1} f$ (where $Z = \sum_{i\in S} f_i$) as $n \to \infty$. Choosing P irreducible and aperiodic, we guarantee the achievement of the convergence to the unique invariant distribution. To make P to have the desired invariant measure f, it suffices to *pick P being in detailed balance with the measure f*, i.e., the transition probabilities should satisfy

$$f_i p_{ij} = f_j p_{ji}.$$

Such a transition matrix is constructed in two steps. As A. Chorin puts it, first do something stupid and then improve it.

(1) Suppose at time n, $X_n = k$. Propose a move from state k according to some irreducible aperiodic transition matrix $Q = (q_{ij})_{ij\in S}$ made-up by you. In the original Metropolis algorithm, the matrix Q must be symmetric, i.e., $q_{ij} = q_{ji}$. Suppose the proposed move is from state k to state l.
(2) To guarantee that the condition $f_i p_{ij} = f_j p_{ji}$ holds, accept the proposed move with the probability

$$\alpha = \min\left\{\frac{f_l}{f_k}, 1\right\}. \tag{13}$$

I.e., if the proposed state l is more likely than the current state k, move to the new state. Otherwise, move there with probability f_l/f_k or stay at state k with probability $1 - f_l/f_k$.

As a result, the transition probabilities p_{ij} are given by

$$p_{ij} = q_{ij} \min\left\{\frac{f_j}{f_i}, 1\right\}, \quad p_{ii} = 1 - \sum_{j\neq i} q_{ij} \min\left\{\frac{f_j}{f_i}, 1\right\}. \tag{14}$$

Let us check that P is in detailed balance with f. Assume $i \neq j$. Let $f_j/f_i \leq 1$. Then

$$f_i p_{ij} = f_i q_{ij} \frac{f_j}{f_i} = f_j q_{ij} = f_j q_{ji} = f_i p_{ji}.$$

If $f_j/f_i > 1$ then

$$f_i p_{ij} = f_i q_{ij} = f_i q_{ji} = f_i p_{ji} \frac{f_j}{f_i} = f_j p_{ij}.$$

Therefore, we have constructed a discrete-time Markov chain converging to the desired equilibrium distribution.

The Metropolis-Hastings algorithm is a generalization of the Metropolis algorithms for the case where the matrix Q is not symmetric, i.e, $q_{ij} \neq q_{ij}$ for at least one pair of states (i, j). It differs from the Metropolis algorithm only by the definition of the acceptance probability α: in the Metropolis-Hastings, α is given by

$$\alpha = \min\left\{\frac{f_l}{f_k}\frac{q_{lk}}{q_{kl}}, 1\right\} \tag{15}$$

Therefore, the transition probabilities p_{ij} are

$$p_{ij} = q_{ij} \min\left\{\frac{f_j}{f_i}\frac{q_{ji}}{q_{ij}}, 1\right\}, \quad p_{ii} = 1 - \sum_{j\neq i} q_{ij} \min\left\{\frac{f_j}{f_i}\frac{q_{ji}}{q_{ij}}, 1\right\}. \tag{16}$$

Exercise Check that $P = (p_{ij})_{i,j\in S}$ and f are in detailed balance.

3.2. **Ising Model.** A description of the Ising model is found in A. Chorin's and O. Hald's book [5] (see sections 5.4 and 5.4 in the 2nd edition). The 2D Ising model is a popular toy example for learning the Metropolis algorithm. Due to its simplicity, and interesting theoretical analysis of this model has been conducted. Numerous internet resources can be readily found. You can find some details regarding its behavior near the critical temperature e.g. here, here, and here.

The Ising model is also considered on other kinds of lattices and on graphs. Variations of the Ising model are used, for example, to model opinion dynamics (e.g., click here and here).

3.3. **MCMC for cryptography.** The Metropolis algorithm can also be used to decipher encrypted messages. A popular description of this application can be found e.g. in P. Diaconis's paper[1].

[1]I thank P. Wertheimer (a graduate student, UMD, MATH) for referring me to cryptography applications of MCMC and this article in particular.

4. Continuous time Markov chains

We will restrict our attention to the case where the set of states S is finite: $|S| = N \in \mathbf{N}$. Consider a weighted directed graph $G(S, E, L)$, were S is the set of vertices, E is the set of arcs (directed edges), and $L = \{L_{ij}\}_{(i\to j)\in E}$ is the set of weights. We assume that there are self-loops of the form $(i \to i)$. Abusing notations, we define the *generator matrix* L as follows:

$$L_{ij} = \begin{cases} L_{ij}, & (i \to j) \in E, \\ 0, & i \neq j, \text{ and } (i \to j) \notin E, \\ -\sum_{k\neq i} L_{ik}, & i = j. \end{cases} \tag{17}$$

Note that the row sums of the matrix L are zero, all off-diagonal entries of L are nonnegative, while all diagonal entries are nonpositive. For convenience, we will denote the sums of off-diagonal entries of row i by L_i, i.e.,

$$L_i := \sum_{j\neq i} L_{ij}. \quad \text{Note that } L_{ii} = -L_i.$$

We define the matrix $P(t)$ for $t \geq 0$ to be the matrix exponential

$$P(t) = e^{tL} := \sum_{k=0}^{\infty} \frac{(tL)^k}{k!}.$$

Exercise Show that

(1) $P(t)$ satisfies the semigroup property:

$$P(s + t) = P(s)P(t) \text{ for all } s, t \geq 0;$$

(2) $P(t)$, $t \geq 0$, satisfies the forward equation

$$\frac{d}{dt}P(t) = P(t)L, \quad P(0) = I;$$

(3) $P(t)$, $t \geq 0$, satisfies the backward equation

$$\frac{d}{dt}P(t) = LP(t), \quad P(0) = I;$$

(4) for $k = 0, 1, 2, \ldots$, we have

$$\left(\frac{d}{dt}\right)^k \Bigg|_{t=0} P(t) = L^k;$$

(5) $P(t)$ is a stochastic matrix for any $t \geq 0$, i.e., its row sums are ones, and all its entries are nonnegative.

Therefore, we can define a discrete-time Markov chain on the graph $G(S, E, L)$ as follows. Pick an interval of time h and an initial probability distribution λ. Then at the moments of time $0,\ h,\ 2h, \ldots$ we will have a discrete-time Markov chain with the initial distribution λ and the transition matrix $P = e^{hL}$.

4.1. **Right-continuous random processes.**

Definition 14.
- *Let S be a discrete set. A continuous-time random process $(X_t)_{t\geq 0}$ with values in S is a family of random variables*
$$X_t : \Omega \to S.$$
- *A random process is right-continuous if for all $\omega \in \Omega$ and all $t \geq 0$ there exists $\epsilon > 0$ such that*
$$X_s(\omega) = X_t(\omega) \text{ for all } t \leq s < t + \epsilon.$$
(I.e., if the system is at state i at time t then there exists an interval of time $[t, t+\epsilon)$ during which the system will stay at i.)

The reason for considering right-continuous random processes is that the probability of any event depending on such a process can be determined in terms of its finite-dimensional distributions, i.e., from the probabilities
$$\mathbb{P}(X_{t_0} = i_0, X_{t_1} = i_1, \ldots, X_{t_n} = i_n)$$
for $n \geq 0$, $0 < t_0 < t_1 < \ldots < t_n$ and $i_0, i_1, \ldots, i_n \in S$.

Definition 15. *The jump times J_0, J_1, ... of $(X_t)_{t\geq 0}$ and holding times S_1, S_2, ... are defined by*
$$J_0 = 0, \quad J_{n+1} = \inf\{t \geq J_n \mid X_t \neq X_{J_n}\}, \quad n = 0, 1, 2, \ldots, \ \inf \emptyset \equiv \infty,$$
$$S_n = \begin{cases} J_n - J_{n-1}, & \text{if } J_{n-1} < \infty, \\ \infty, & \text{otherwise} \end{cases}.$$

4.2. **The exponential distribution.** We interpret the absolute values of the diagonal entries of the generator matrix L as the escape rates: L_i is the escape rate from the state i. Correspondingly, if $L_i > 0$, L_i^{-1} is the expected holding time at state i. The off-diagonal entries L_{ij}, $i \neq j$ of L are often called the pairwise transition rates.

Now we will go over some important properties of exponential random variables. Suppose the jump time T from i to j is an exponentially distributed random variable with parameter L_i, i.e.,
$$\mathbb{P}(T > t) = e^{-L_i t} \quad \text{for all } t \geq 0.$$
If $L_i > 0$, then T has pdf
$$f_T(t) = \begin{cases} L_i e^{-L_i t}, & t \geq 0, \\ 0, & t < 0. \end{cases}$$
The expected value of T is
$$E[T] = \int_0^\infty L_i e^{-L_i t} t dt = \frac{1}{L_i},$$
i.e., L_i is the reciprocal of the expected jump time.

Why did we choose the exponential distribution for the jump times? The reason is that the exponential random variable is the only random variable that possesses the *memoryless property*.

Theorem 13. *A random variable $T : \Omega \to [0, \infty]$ has an exponential distribution if and only if it has the following memoryless property:*

$$\mathbb{P}(T > t + s \mid T > s) = \mathbb{P}(T > t) \text{ for all } s, t \geq 0. \tag{18}$$

Exercise Prove it.

Exercise Show that if T is an exponential random variable with parameter λ and $a > 0$ then $\frac{T}{a}$ is an exponential random variable with parameter λa.

Theorem 14. *Let S be a countable set and let T_k, $k \in S$, be independent exponential random variables with parameters q_k. Let*

$$0 < q := \sum_{k \in S} q_k < \infty.$$

Set

$$T := \inf_{k \in S} T_k.$$

Then this infimum is attained at a unique random value $K \in S$, with probability 1. Moreover, T and K are independent, and T is exponential with parameter q, and

$$\mathbb{P}(K = k) = \frac{q_k}{q}.$$

Proof. Set $K = k$ if $T_k < T_j$ for all $j \neq k$, otherwise let K be undefined. Then

$$\begin{aligned}
\mathbb{P}(K = k \ \& \ T > t) &= \mathbb{P}(T_k > t \ \& \ T_j > T_k \text{ for all } j \neq k) \\
&= \int_t^\infty q_k e^{-q_k s} \mathbb{P}(T_j > s \text{ for all } j \neq k) ds \\
&= \int_t^\infty q_k e^{-q_k s} \prod_{j \neq k} e^{-q_j s} ds \\
&= \int_t^\infty q_k e^{-qs} ds = \frac{q_k}{q} e^{-qt}.
\end{aligned}$$

Hence

$$\mathbb{P}(K = k \text{ for some } k) = 1$$

and T and K have the claimed joint distribution. □

4.3. **Jump chains and holding times.** Given a generator matrix L one can define the *jump matrix* $\Pi = (\pi_{ij} \mid i, j \in S)$ as follows:

$$\pi_{ij} = \begin{cases} \frac{L_{ij}}{L_i}, & i \neq j \text{ and } L_i \neq 0, \\ 0, & i \neq j \text{ and } L_i = 0 \end{cases}, \qquad \pi_{ii} = \begin{cases} 0, & L_i \neq 0, \\ 1, & L_i = 0 \end{cases}. \tag{19}$$

Now we can give a definition of a continuous-time Markov chain in terms of its jump chain and holding times.

Definition 16. *A right-continuous process $(X_t)_{t\geq 0}$ on S is a continuous-time Markov chain with initial distribution λ and generator matrix L if its jump chain is discrete-time Markov chain $(Y_n)_{n\geq 0}$ with initial distribution λ and transition matrix Π defined from L by Eq. (19) and if for each $n \geq 1$, conditional on Y_0, ..., Y_{n-1}, its holding times S_1, ..., S_n are independent exponential random variables with parameters L_{Y_0}, ..., $L_{Y_{n-1}}$ respectively.*

Given a discrete-time Markov chain $(Y_n)_{n\geq 0}$ with initial distribution λ and transition matrix Π, and independent random variables $T_1, T_2, \ldots$ with parameter 1, one can construct a continuous time random chain $(X_t)_{t\geq 0}$ with the same set of states and the same initial distribution as follows. Set the holding times and the jump times according to:

$$S_n = \frac{T_n}{L_{Y_{n-1}}}, \qquad J_n = S_1 + \ldots + S_n.$$

Then define

$$X_t = Y_n \quad \text{where } n \text{ is such that } J_n \leq t < J_{n+1}.$$

Given a continuous-time Markov chain $(X_t)_{t\geq 0}$ with initial distribution λ and generator matrix L, one can construct a discrete-time random chain $(Y_n)_{n\geq 0}$ with the same set of states and the same initial distribution as follows. We begin with an initial state $X_0 = Y_0$ with distribution λ, and with an array $(T_n^j \mid n \geq 1, j \in S)$ of independent exponential random variables with parameter 1. Then, inductively, for $n = 0, 1, 2, \ldots$, if $Y_n = i$ we set

$$S_{n+1}^j = \frac{T_{n+1}^j}{L_{ij}}, \quad \text{for } j \neq i, \tag{20}$$

$$S_{n+1} = \inf_{j\neq i} S_{n+1}^j, \tag{21}$$

$$Y_{n+1} = j = \arg\min_{j\neq i} S_{n+1}^j. \tag{22}$$

Then, conditional on $Y_n = i$, the random variables S_{n+1}^j are independent exponential random variables with parameters L_{ij} for all $j \neq i$. So, conditional on $Y_n = i$, S_{n+1} is exponential with parameter $L_i = \sum_{j\neq i} L_{ij}$. Furthermore, Y_{n+1} has distribution $(\pi_{ij} \mid j \in S)$, and S_{n+1} and Y_{n+1} are independent, and independent of Y_0, ..., Y_n and S_1, ..., S_n as required. This construction shows why we call L_i the rate of leaving i (or the escape rate from i) and L_{ij} the rate of going for i to j (or the transition rate from i to j).

Example 8 Let us convert the continuous-time Markov chain in Fig. 4 (left) to a corresponding jump chain. The result is shown in Fig. 4 (right). The continuous-time Markov chain on the right has the generator matrix L given by

$$L = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 7 & -15 & 2 & 6 \\ 0 & 1 & -5 & 4 \\ 0 & 5 & 3 & -8 \end{bmatrix}.$$

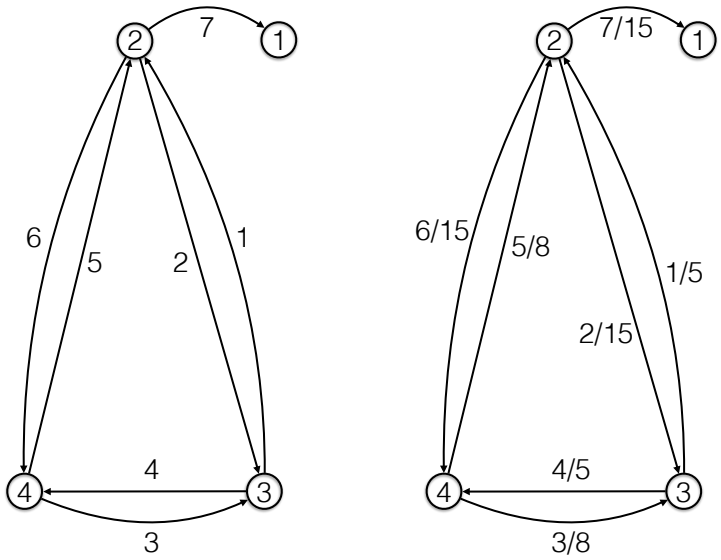


FIGURE 4. Conversion of a continuous-time Markov chain (left) into the corresponding jump chain (right). The jump rates are calculated the pairwise transition rates using Eq. (19).

Using Eq. (19) we calculate the jump rates for the corresponding jump chain on the right:

$$\Pi = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 7/15 & 0 & 2/15 & 6/15 \\ 0 & 1/5 & 0 & 4/5 \\ 0 & 5/8 & 3/8 & 0 \end{bmatrix}.$$

Note that the any jump chain is a discrete-time Markov chain, where the probability to stay at any state unless it is an absorbing state is zero. Vice versa, given a jump matrix Π and the escape rates L_i, $i \in S$, one can construct the generator matrix L for the corresponding continuous-time Markov chain.

Theorem 15. *Let $(X_t)_{t\geq 0}$ be a right-continuous random process with values in a finite set S. Let L be a generator matrix on S with jump matrix Π. Then the following three conditions are equivalent:*

(1) **(jump chain/holding time definition)** *conditional on $X_0 = i$, the jump chain $(Y_n)_{n\geq 0}$ of $(X_t)_{t\geq 0}$ is a discrete-time Markov chain and for each $n \geq 1$, conditional on Y_0, ..., Y_{n-1}, the holding times S_1, ..., S_n are independent exponential random variables with parameters L_{Y_0}, ..., $L_{Y_{n-1}}$ respectively;*

(2) **(infinitesimal definition)** *for all $t, h \geq 0$, conditional on $X_t = i$, X_{t+h} is independent of $(X_s \mid s < t)$ and, as $h \downarrow 0$, uniformly in t, for all j*

$$\mathbb{P}(X_{t+h} = j \mid X_t = i) = \delta_{ij} + L_{ij}h + o(h),$$

where δ_{ij} is the Kronecker symbol:

$$\delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

(3) **(transition probability definition)** *for all $n = 0, 1, 2, \ldots$, all times $0 < t_0 < t_1 < \ldots < t_{n+1}$ and all states $i_0, \ldots, i_{n+1}$*

$$\begin{aligned} \mathbb{P}(X_{t_{n+1}} = i_{n+1} \mid X_{t_0} = i_0, \ldots, X_{t_n} = i_n) &= \mathbb{P}(X_{t_{n+1}} = i_{n+1} \mid X_{t_n} = i_n) \\ &= p_{i_n i_{n+1}}(t_{n+1} - t_n), \end{aligned} \tag{23}$$

where $\{p_{ij}(t) \mid i, j \in S,\ t \geq 0\}$ is the solution of the forward equation

$$P'(t) = P(t)L,\ P(0) = I.$$

If $(X_t)_{t\geq 0}$ satisfies any of these three conditions, we say that it is a continuous-time Markov chain with the generator matrix L.

Proof. (1) Suppose (1) holds and prove (2). As $h \downarrow 0$,

$$\mathbb{P}_i(X_h = i) \geq \mathbb{P}_i(J_1 > h) = e^{-L_i h} = 1 + L_{ii}h + o(h),$$

(recall that $L_{ii} = -L_i$), and for $j \neq i$,

$$\begin{aligned} \mathbb{P}_i(X_h = j) &\geq \mathbb{P}_i(J_1 \leq h,\ Y_1 = j,\ S_2 > h) \\ &= (1 - e^{-L_i h})\pi_{ij} e^{-L_j h} = L_{ij}h + o(h). \end{aligned}$$

Thus, for every state j there is an inequality

$$\mathbb{P}_i(X_h = j) \geq \delta_{ij} + L_{ij}h + o(h).$$

By taking the finite sum over j we see that these must be equalities: the left-hand sides sum up to 1 while the right-hand sides sum up to $1 + o(h)$. Then, by Markov property, for any $t, h \geq 0$, conditional on $X_t = i$, X_{t+h} is independent of $(X_s \mid s \leq t)$ and, as $h \downarrow 0$, uniformly in t

$$\mathbb{P}(X_{t+h} = j \mid X_t = i) = \mathbb{P}_i(X_h = j) = \delta_{ij} + L_{ij}h + o(h).$$

(2) Suppose (2) holds and prove (3). Set $p_{ij}(t) = \mathbb{P}_i(X_t = j) = \mathbb{P}(X_t = j \mid X_0 = i)$. For all $t, h \geq 0$, as $h \downarrow 0$, uniformly in t

$$\begin{aligned} p_{ij}(t + h) &= \sum_{k \in S} \mathbb{P}_i(X_t = k)\mathbb{P}(X_{t+h} = j \mid X_t = k) \\ &= \sum_{k \in S} p_{ik}(t)(\delta_{kj} + L_{kj}h + o(h)). \end{aligned}$$

Since S is finite we have

$$\frac{p_{ij}(t+h)-p_{ij}(t)}{h}=\sum_{k\in S}p_{ik}(t)L_{kj}+o(1).$$

So, letting $h\downarrow 0$, we see that $p_{ij}(t)$ is differentiable on the right. Then by uniformity we replace t by $t-h$ in the above and let $h\downarrow 0$ to see first that $p_{ij}(t)$ is continuous on the left, then differentiable on the left, hence differentiable, and satisfies the forward equations

$$p'_{ij}(t)=\sum_{k\in S}p_{ik}(t)L_{kj},\ p_{ij}(0)=\delta_{ij}.$$

Since S is finite, $p_{ij}(t)$ is the unique solution of the forward equation. Also, if (2) holds then Eq. (23) holds.

(3) Suppose (3) holds and prove (1). Condition (3) determines the finite-dimensional distributions of $(X_t)_{t\geq 0}$ and hence the distribution of jump chain and holding times. Hence condition (1) is satisfied.

□

4.4. **Class structure.** The concepts *i leads to j* ($i\longrightarrow j$), *i communicates with j* ($i\longleftrightarrow j$), *communicating class, closed class, absorbing state*, and *irreducibility* are inherited from discrete-time Markov chains.

Theorem 16. *For distinct states $i,j\in S$ the following are equivalent:*

(1) $i\longrightarrow j$;
(2) $i\longrightarrow j$ *for the jump chain;*
(3) $L_{ii_1}L_{i_1i_2}\dots L_{i_{n-1}j}>0$ *for some states i_1, ..., i_{n-1};*
(4) $p_{ij}(t)>0$ *for all $t>0$;*
(5) $p_{ij}(t)>0$ *for some $t>0$.*

Proof. Implications (4) $\Rightarrow$ (5) $\Rightarrow$ (1) $\Rightarrow$ (2) are clear. If (2) holds then there are states

$$i_1,\dots,i_{n-1}\text{ such that }\pi_{ii_1}\pi_{i_1i_2}\dots\pi_{i_{n-1}j}>0,$$

which implies (3).

If $L_{ij}>0$, then

$$p_{ij}(t)\geq\mathbb{P}_i(J_1\leq t,Y_1=j,S_2>t)=(1-e^{-L_it})\pi_{ij}e^{-L_jt}>0\text{ for all }t.$$

So, if (3) holds, then

$$p_{ij}(t)\geq p_{ii_1}(t/n)p_{i_1i_2}(t/n)\dots p_{i_{n-1}j}(t/n)>0\text{ for all }t.$$

Hence (4) holds. □

4.5. **Hitting times and absorption probabilities.**

Definition 17. *Let $(X_t)_{t\geq 0}$ be a Markov chain with generator matrix L. The hitting time of a subset $A \subset S$ is the random variable*

$$\tau^A(\omega) = \inf\{t \geq 0 \mid X_t(\omega) \in A\}$$

with the usual convention $\inf \emptyset = \infty$.

The probability that, starting from i, $(X_t)_{t\geq 0}$ ever hits A is then

$$h_i^A = \mathbb{P}_i(\tau^A < \infty).$$

When A is a closed class, h_i^A is called the *absorption probability*.

Note that the hitting probabilities are the same as in the jump chain. Therefore, we can calculate them as we have done it for discrete-time Markov chains.

Theorem 17. *The vector of hitting times is the minimal nonnegative solution of*

$$\begin{cases} h_i^A = 1, & i \in A, \\ \sum_{j\in S} L_{ij} h_j^A = 0, & i \notin A. \end{cases} \tag{24}$$

Proof. Since the hitting probabilities are the same for continuous-time Markov chains and the corresponding jump chains, we will start with Eq. (4) where π_{ij} are the transition probabilities. Consider $i \notin A$. First assume $L_i > 0$. Then $\pi_{ij} = L_{ij}/L_i$ and $\pi_{ii} = 0$. Then, taking into account that $L_{ii} = -L_i$ and $L_i = \sum_{j\neq i} L_{ij}$ we have:

$$h_i^A = \sum_{j\in S} \pi_{ij} h_j^A = \sum_{j\neq i} \frac{L_{ij}}{L_i} h_j^A = \sum_{j\neq i} \frac{L_{ij}}{L_i} h_j^A + h_i^A \frac{L_{ii}}{L_i} + h_i^A.$$

Canceling h_i^A in the right- and left-hand side and then canceling L_i we get

$$\sum_{j\in S} L_{ij} h_j^A = 0.$$

If $L_i = 0$ then i is an absorbing state. Then $\pi_{ii} = 1$, $\pi_{ij} = 0$ for $j \neq i$. Then Eq. (4) gives $h_i^A = h_i^A$ while Eq. (24) gives $0 = 0$. □

The mean hitting times k_i^A are defined as they were for discrete-time chains.

$$k_i^A = E_i[\tau^A] = E[\tau^A \mid X_0 = i]$$

Theorem 18. *Assume that $L_i > 0$ for all $i \notin A$. The vector of mean hitting times $k^A = \{k_i^A \mid i \in S\}$ is the minimal nonnegative solution of*

$$\begin{cases} k_i^A = 0, & i \in A, \\ \sum_{j\in S} L_{ij} k_j^A = -1, & i \notin A. \end{cases} \tag{25}$$

The proof follows the same lines as the one for the case of discrete-time Markov chains. Here we will verify that Eq. (25) must be satisfied. If $X_0 \in A$ then $\tau^A = 0$ and hence $k_i^A = 0$. If $X_0 \notin A$ then $\tau^A \geq J_1$, so, by Markov property of the jump chain

$$E_i[\tau^A - J_1 \mid Y_1 = j] = E_j[\tau^A].$$

Therefore,

$$\begin{aligned} k_i^A = E_i[\tau^A] &= E_i[J_1] + \sum_{j \neq i} E_i[\tau^A - J_1 \mid Y_1 = j]\mathbb{P}_i(Y_1 = j) \\ &= L_i^{-1} + \sum_{j \neq i} \pi_{ij} k_j^A \\ &= L_i^{-1} + \sum_{j \neq i} \frac{L_{ij}}{L_i} k_j^A = L_i^{-1} + \sum_{j \in S} \frac{L_{ij}}{L_i} k_j^A + k_i^A. \end{aligned}$$

Canceling k_i^A and then L_i, we obtain

$$\sum_{j \in S} L_{ij} k_j^A + 1 = 0$$

Which implies Eq. (25).

4.6. **Recurrence and transience.** We say that a state i is recurrent if

$$\mathbb{P}_i(\{t \geq 0 \mid X_t = i\} \text{ is unbounded}) = 1.$$

We say that a state i is transient if

$$\mathbb{P}_i(\{t \geq 0 \mid X_t = i\} \text{ is unbounded}) = 0.$$

Theorem 19. *Let $(X_t)_{t \geq 0}$ be a Markov chain with generator matrix L, and $(Y_n)_{n \geq 0}$ be the corresponding jump chain.*

1. *If i is recurrent for the corresponding jump chain $(Y_n)_{n \geq 0}$ then i is recurrent for the continuous-time chain $(X_t)_{t \geq 0}$.*
2. *If i is transient for the corresponding jump chain $(Y_n)_{n \geq 0}$ then i is transient for the continuous-time chain $(X_t)_{t \geq 0}$.*
3. *Every state is either transient or recurrent.*
4. *Recurrence and transience are class properties.*

The first passage time to i is defined by

$$T_i(\omega) = \inf\{t \geq J_1(\omega) \mid X_t(\omega) = i\}.$$

Theorem 20. *The following dichotomy holds:*

1. *if $L_i = 0$ or $\mathbb{P}_i(T_i < \infty) = 1$, then i is recurrent and $\int_0^\infty p_{ii}(t)dt = \infty$;*
2. *if $L_i > 0$ and $\mathbb{P}_i(T_i < \infty) < 1$, then i is transient and $\int_0^\infty p_{ii}(t)dt < \infty$.*

4.7. **Invariant distributions and convergence to equilibrium.** Since we are considering only Markov chains where the set of states is finite, all invariant measures can be normalized so that the sum of their entries is one, and therefore, every invariant measure can be made into an invariant distribution.

Definition 18. *We say that* $\lambda = \{\lambda_i \mid i \in S\}$ *is an invariant measure if* $\lambda_i \geq 0$ *for all* i*,*

$$\lambda L = 0.$$

Theorem 21. *Let* L *be the generator matrix and let* λ *be a measure. Then the following are equivalent:*

(1) λ *is invariant;*
(2) $\mu\Pi = \mu$ *where* $\mu_i = \lambda_i L_i$.

Proof. Recall:

- $\pi_{ij} = L_{ij}/L_i$ if $i \neq j$ and $L_i > 0$;
- $\pi_{ij} = 0$ if $i \neq j$ and $L_i = 0$;
- $\pi_{ii} = 0$ if $L_i > 0$;
- $\pi_{ii} = 1$ if $L_i = 0$.

This can be written as in one line as

$$L_i(\pi_{ij} - \delta_{ij}) = L_{ij}.$$

The equality $\mu = \mu\Pi$ is equivalent to $\mu(\Pi - I) = 0$. We have

$$(\mu(\Pi - I))_j = \sum_{i \in S} \mu_i(\pi_{ij} - \delta_{ij}) = \sum_{i \in S} \lambda_i L_i(\pi_{ij} - \delta_{ij}) = \sum_{i \in S} \lambda_i L_{ij} = (\lambda L)_j.$$

This proves the theorem. □

Theorem 22. *Let* L *be an* $N \times N$ *irreducible generator matrix, and* λ *be a measure. Let* $s > 0$ *be given. Then the following are equivalent:*

(1) $\lambda L = 0$*;*
(2) $\lambda P(s) = \lambda$.

Proof. By the backward equation

$$\frac{d}{ds}\lambda P(s) = \lambda \frac{d}{ds} P(s) = \lambda L P(s).$$

Hence $\lambda L = 0$ implies

$$\lambda P(s) = \lambda P(0) = \lambda I = \lambda \text{ for all } s.$$

On the other hand, $\lambda P(s) = \lambda$ implies that $\frac{d}{ds}\lambda P(s) = 0$. Since $P(s)$ is invertible as it is the fundamental solution matrix of a first order linear differential equation with constant coefficients, $\lambda L P(s) = 0$ implies that $\lambda L = 0$.

□

Theorem 23. *Let* L *be an* $N \times N$ *irreducible generator matrix. Then there exists a unique invariant distribution* π *and for all states* $i, j \in S$

$$\lim_{t \to \infty} p_{ij}(t) = \pi_j.$$

Proof. Existence and uniqueness of the invariant distribution follows from its existence and uniqueness for the matrix $P(t) = e^{tL}$. Let us show this.

All entries of $P(t)$ are positive for all $t > 0$ owing to irreducibility and Theorem 16. Applying the Perron-Frobenius theorem (Theorem 8) we conclude that $P(t)$ has an eigenvalue $\mu_0 = 1$ whose algebraic multiplicity is equal to 1 and $\mu_0 > |\mu_k|$ for all other eigenvalues μ_k of P. The unique invariant distribution π is the left eigenvector of $P(t)$ corresponding to the eigenvalue $\mu_0 = 1$, i.e.,

$$\pi = \pi P(t).$$

By Theorem 22, this is equivalent to $\pi L = 0$. Hence there exists a unique invariant distribution π such that $\pi L = 0$.

Now we will show convergence to π. We conduct the proof for the case when L is diagonalizable. It it is not, the proof is similar but a bit more tedious (see the proof of the analogous theorem (Theorem 9) for discrete-time Markov chains.) Let $\lambda_0 = 0,\ \lambda_1,\ \ldots,\ \lambda_{N-1}$ be eigenvalues of L. If

$$L = V\Lambda U$$

is the eigendecomposition of L then $P(t)$ has the eigendecomposition

$$P(t) \equiv e^{tL} = V \begin{bmatrix} 1 & & & \\ & e^{\lambda_1 t} & & \\ & & \ddots & \\ & & & e^{\lambda_{N-1} t} \end{bmatrix} U.$$

Therefore, the eigenvalues of $P(t)$ are

$$\mu_0 = 1,\ \mu_1 = e^{\lambda_1 t}, \ldots, \mu_{N-1} = e^{\lambda_{N-1} t}.$$

Since $|\mu_k| < 1$ for $1 \le k \le N-1$, we conclude that the real parts of λ_k, $k = 1, 2, \ldots, N-1$ are negative, i.e.,

$$Re(\lambda_k) < 0 \text{ for } k = 1, 2, \ldots, N-1.$$

Hence

$$\lim_{t\to\infty} e^{\lambda_k t} = 0 \text{ for } k = 1, 2, \ldots, N-1.$$

V is the matrix of right eigenvectors of L. Since row sums of L are zeros, the first eigenvector corresponding to the zero eigenvalue, i.e. the first column of V, must be $e = [1\ 1\ \ldots\ 1]^\top$. The first row of U, the matrix of left eigenvectors of L must be the invariant distribution π. We will denote the rest of right eigenvectors by v_k and the rest of left eigenvectors by ϕ_k, i.e.,

$$V = [e\ v_1\ \ldots v_{N-1}], \quad U = \begin{bmatrix} \pi \\ \phi_1 \\ \vdots \\ \phi_{N-1} \end{bmatrix}.$$

Then

$$P(t) = [e\ v_1\ \dots v_{N-1}] \begin{bmatrix} 1 & & & \\ & e^{\lambda_1 t} & & \\ & & \ddots & \\ & & & e^{\lambda_{N-1} t} \end{bmatrix} \begin{bmatrix} \pi \\ \phi_1 \\ \vdots \\ \phi_{N-1} \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} [\pi_1\ \dots\ \pi_N] + \sum_{k=1}^{N-1} v_k e^{\lambda_k t} \phi_k \tag{26}$$

$$\to \begin{bmatrix} \pi_1 & \dots & \pi_N \\ \vdots & & \vdots \\ \pi_1 & \dots & \pi_N \end{bmatrix} \text{ as } t \to \infty.$$

□

4.8. **Time reversal and detailed balance for continuous-time Markov chains.** For continuous-time Markov chains analogous results for time reversal and detailed balance take place. Let L be an irreducible generator matrix and π be an invariant distribution. The generator matrix $\hat{L}$ for the time-reversal is defined by

$$\pi_i \hat{L}_{ij} = \pi_j L_{ji}.$$

The detailed balance condition reads

$$\pi_i L_{ij} = \pi_j L_{ji}.$$

Analogs of Theorems 10, 11, 12 hold.

5. Transition Path Theory

The Transition Path Theory (TPT) was introduced by W. E and E. Vanden-Eijnden in 2006 [10, 11] in the context of stochastic differential equations. They contraposed it to the Transition State Theory (TST) developed by Eyring and Polanyi in 1930s. In a nutshell, TPT is a conceptual apparatus for describing reactive events. The key concept of the TPT, the committor function, is a solution of a boundary value problem of a certain elliptic PDE. It cannot be solved in practice in dimensions higher than 3 by means of finite difference or finite element methods. However, recent successes in solving PDEs by means of neural networks did open new horizons.

Metzner, Schuette, and Vanden-Eijnden (2009) [14] extended TPT to continuous-time Markov chains (a.k.a Markov jump processes (MJP)). Since the application of the TPT to MJP is hinged to finding the committor that, in this case, is the solution to a system of linear algebraic equations which, in practice, can be either readily done or done after some additional work, the TPT has become a powerful practical tool for analysis of transition processes in complex networks. For example, one of the benchmark problems in chemical physics, the rearrangement of the Lennard-Jones cluster of 38 atoms was analyzed using

the TPT and resulted in a detailed description of the transition mechanism between the two lowest potential energy minima [8].

5.1. **Settings.** We will consider a continuous-time Markov chain with a finite set of states S, $|S| = N$, and irreducible generator matrix L. This Markov chain can be represented as a network, where states correspond to the vertices of the graph, two vertices i and j are connected by a directed edge if an only if $L_{ij} > 0$. If both $L_{ij} > 0$ and $L_{ji} > 0$, we will draw an undirected edge between i and j.

Let A and B be selected nonintersecting subsets of S. For simplicity, we assume that there exists no edge (i, j) such that $i \in A$ and $j \in B$, i.e., one cannot get from A to B without spending some time in $S\backslash(A\cup B) \equiv (A\cup B)^c$. The sets A and B can be interpreted as the reactant set and the product set respectively. For example, if you are modeling a protein folding, A can be a collection of unfolded states, while B – a collection of folded states.

There exists a unique invariant distribution $\pi = (\pi_i)_{i\in S}$, i.e., $\pi L = 0$. **We do not assume that π and L are in detailed balance**. We will also need to consider a family of time reversed chains $(\hat{X}_t)_{t\in\mathbb{R}}$, $\hat{X}_t = X_{\tau-t}$ where τ is some moment of time. The generator matrix for the time reversed process is $\hat{L} = (\hat{L}_{ij})_{i,j\in S}$ defined by

$$\hat{L}_{ij} = \frac{\pi_j}{\pi_i} L_{ji}.$$

5.2. **Reactive trajectories.** The subject of TPT is reactive trajectories that are defined as follows. Consider a very long trajectory starting from an arbitrary state i, i.e., $(X_t)_{t\in\mathbb{R}}$ such that $X_0 = i$. Since the Markov chain is irreducible and finite, every state is recurrent. Hence this trajectory will visit all of the states infinitely many times with probability 1. Let us prune those pieces of it that go from A to B, i.e., we will detect the collections of moments of time $\{t_n^A\}_{n\in\mathbb{N}}$ and $\{t_n^B\}_{n\in\mathbb{N}}$ such that

$$t_n^A < t_n^B < t_{n+1}^A \quad n \in \mathbb{N},$$

$$\lim_{t\uparrow t_n^A} X(t) = x_n^A \in A, \quad X(t_n^B) = x_n^B \in B,$$

$$\text{for any } t \in [t_n^A, t_n^B)\ X(t) \in (A \cup B)^c.$$

In words, t_n^A is the moment of time when the trajectory leaves A nth time so that it does not return to A prior reaching B, and t_n^B is the nth time when the trajectory enters B. The intervals $[t_n^A, t_n^B)$ are called *reactive times*. The union of the reactive times is denoted by R:

$$R := \bigcup_{n\in\mathbb{Z}} (t_n^A, t_n^B).$$

Now consider the corresponding jump chain and the jump trajectory $(Y_k)_{k\geq 0}$.

Definition 19. *The ordered sequence*

$$\phi_n = [x_n^A, x_n^1, \ldots, x_n^{k_n} \equiv x_n^B]$$

consisting of successive states of the jump chain $(Y_k)_{k\in\mathbb{Z}}$ visited during the nth transition from A to B is called the nth reactive trajectory. The set of all such sequences is called the set of reactive trajectories.

The concept of reactive trajectory is illustrated in Fig. 5.

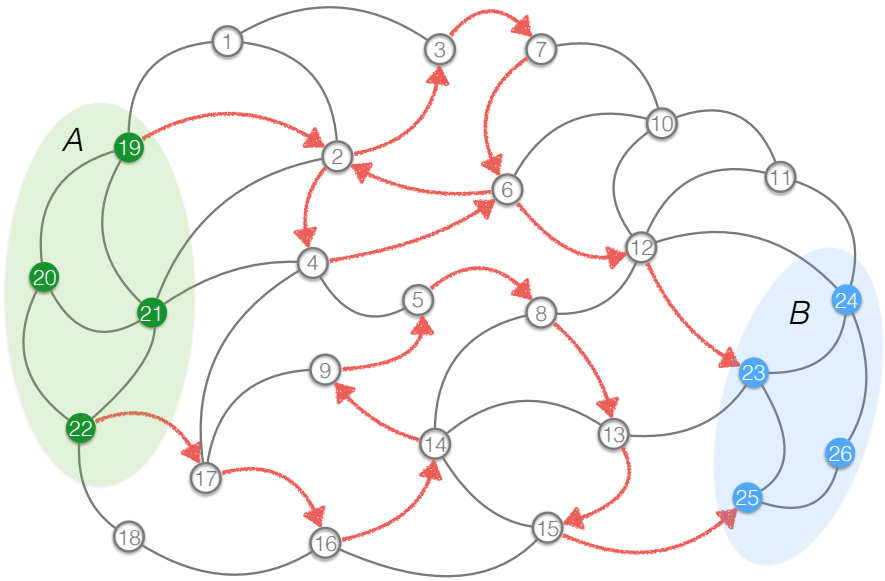


FIGURE 5. Two examples of reactive trajectories are shown in red. Reactive trajectory 1: $[19, 2, 3, 7, 6, 2, 4, 6, 12, 23]$. Reactive trajectory 2: $[22, 17, 16, 14, 9, 5, 8, 13, 15, 25]$.

5.3. **The forward and backward committors.**

Definition 20. *The forward committor $q^+ = (q_i^+)_{i\in S}$ is the probability that the process starting at state i will first reach B rather than A, i.e.,*

$$q_i^+ = \mathbb{P}_i(\tau_B^+ < \tau_A^+),$$

where

$$\tau_A^+ = \inf\{t > 0 \mid X(t) \in A\}, \quad \tau_B^+ = \inf\{t > 0 \mid X(t) \in B\}$$

are the first entrance times to A and B respectively.

The backward committor $q^- = (q_i^-)_{i\in S}$ is the probability that the process arriving at state i last came from A rather than B. Equivalently, the backward committor $q^- = (q_i^-)_{i\in S}$ is

the probability that the time-reversed process starting at state i will first reach B rather than A, i.e.,

$$q_i^- = \mathbb{P}_i(\tau_A^- < \tau_B^-),$$

where

$$\tau_A^- = \inf\{t > 0 \mid \hat{X}(t) \in A\}, \quad \tau_B^- = \inf\{t > 0 \mid \hat{X}(t) \in B\},$$

are the last exit times from A and B respectively. Here $(\hat{X}_t)_{t\in\mathbb{R}}$ is the time-reversed process for $(X_t)_{t\in\mathbb{R}}$, i.e., $\hat{X}_t = X_{-t}$, $t \in \mathbb{R}$.

The forward and backward committors satisfy the following equations:

$$\begin{cases} \sum_{j\in S} L_{ij} q_j^+ = 0, & i \in (A \cup B)^c, \\ q_i^+ = 0, & i \in A, \\ q_i^+ = 1, & i \in B, \end{cases} \tag{27}$$

and

$$\begin{cases} \sum_{j\in S} \hat{L}_{ij} q_j^- = 0, & i \in (A \cup B)^c, \\ q_i^- = 1, & i \in A, \\ q_i^- = 0, & i \in B, \end{cases} \tag{28}$$

where $\hat{L}$ is the generator matrix for the time-reversed process.

Eq. (27) is justified as follows. Let us modify out network and make all states in A absorbing, i.e., $L_{ij} = 0$ for all $i \in A$. The other L_{ij}'s are unchanged. Then Eq. (27) becomes the equation for the hitting probabilities for the set B for the modified network. I. e., q_i^+ is the probability that the process starting at i will hit B prior being absorbed by one of the states in A. This is exactly what the forward committor is. A similar argument applied to the reversed process shows that the backward committor satisfies Eq. (28).

5.4. **Probability distribution of reactive trajectories.** What is the probability to find a reactive trajectory at state i at any time t? To answer this question, consider an infinitely long trajectory $(X_t)_{t\in\mathbb{R}}$ where X_0 is distributed according to the invariant distribution π. For any fixed time t, the probability to find X_t at state i is π_i. If $X_t = i$ where $i \in A$ or $i \in B$, time t is not reactive, hence this probability is 0. If $X_t = i$ where $i \in (A \cup B)^c$, we need to take the probability π_i to find X_t at i and multiply it by the probability that X_t came to i from A and will go next to B, i.e., by $q_i^- q_i^+$. Therefore, the probability to find a reactive trajectory at state i at any time t is given by

$$m_i^R = \pi_i q_i^- q_i^+. \tag{29}$$

In [14], m_i^R is called the probability distribution of reactive trajectories. Note that m^R is not a distribution, as it is not normalized. It is a measure. The normalization constant for m_i^R,

$$Z_R = \sum_{i\in S} m_i^R = \sum_{i\in S} \pi_i q_i^- q_i^+,$$

is the probability that any given t belongs to the set of reactive times, i.e.,

$$Z_R = \mathbb{P}(t \in \bigcup_{n\in\mathbb{Z}} (t_n^A, t_n^B)) \equiv \mathbb{P}(t \in R).$$

5.5. **Probability current of reactive trajectories.** The probability current of reactive trajectories along edge $(i \to j)$ is defined as the average number of transitions for i to j per unit time performed by reactive trajectories. This probability current denoted by f_{ij} is given by

$$f_{ij} = \begin{cases} \pi_i q_i^- L_{ij} q_j^+, & i \neq j, \\ 0, & i = j. \end{cases} \tag{30}$$

Indeed, the product $\pi_i q_i^-$ gives the probability that the trajectory arrived at i from A rather than from B. L_{ij} is the transition rate from i to j, and the factor q_j^+ is the probability that the trajectory from j will go next to B rather than to A.

It follows from Eq. (30) that the probability current of reactive trajectories along every edge (i, j) is nonnegative. Note that for an edge (i, j) where $i, j \in (A \cup B)^c$ both f_{ij} and f_{ji} can be positive. This reflects the fact that reactive trajectories can go many times back and forth across the edge (i, j) on their way from A to B. The next theorem says that the probability current in neither produced nor absorbed at any state $j \in (A \cup B)^c$.

Theorem 24. *For all $i \in (A \cup B)^c$, the probability current is conserved, i.e., the amount of current coming to state i equals to the amount of current going out of state i:*

$$\sum_{j\in S} (f_{ij} - f_{ji}) = 0 \text{ for all } i \in (A \cup B)^c. \tag{31}$$

Proof. Let $i \in (A \cup B)^c$. Plugging in Eq. (30) to Eq. (31) we obtain

$$\begin{aligned} \sum_{j\in S} (f_{ij} - f_{ji}) &= \sum_{j\neq i} (\pi_i q_i^- L_{ij} q_j^+ - \pi_j q_j^- L_{ji} q_i^+) \\ &= \pi_i q_i^- \sum_{j\neq i} L_{ij} q_j^+ - q_i^+ \sum_{j\neq i} \pi_j L_{ji} q_j^-. \end{aligned}$$

It follows from Eqs. (27) and (28) that

$$\sum_{j\neq i} L_{ij} q_j^+ = L_i q_i^+$$

and

$$\sum_{j\neq i} \pi_j L_{ji} q_j^- = \sum_{j\neq i} \frac{\pi_i}{\pi_j} \pi_j \hat{L}_{ij} q_j^- = \pi_i \hat{L}_i q_i^- = \pi_i L_i q_i^-.$$

Therefore,

$$\sum_{j\in S} (f_{ij} - f_{ji}) = \pi_i q_i^- L_i q_i^+ - q_i^+ \pi_i L_i q_i^- = 0.$$

□

5.6. **Effective current.** As we have mentioned, the reactive trajectories can go back in forth along an edge (i,j) where $i,j \in (A\cup B)^c$ on their way from A to B making both f_{ij} and f_{ji} positive. The difference $f_{ij}-f_{ji}$ is the net current from i to j carried by reactive trajectories from i to j. The nonnegative part of $f_{ij}-f_{ji}$, denoted by f_{ij}^+, is called the *effective current*:

$$f_{ij}^+ := \max\{f_{ij}-f_{ji},0\}. \tag{32}$$

Note that the effective current for time-irreversible Markov chains can be cyclic. Indeed, the probability current of reactive trajectories contains all kinds of cycles, and going to effective current removes only all cycles of of length 2, but not of length 3, 4, etc. In contrast, effective current for reversible Markov chains is acyclic. We will discuss this in more details below.

5.7. **Transition rate.** The transition rate from A to B (the reaction rate) is the average number of transitions per unit time performed by an infinite trajectory $(X_t)_{t\in\mathbb{R}}$. It is equal to the total reactive current coming out of A which is the same as the total reactive current going into B, i.e.,

$$\begin{aligned}\nu_R &= \sum_{i\in A,\ j\in S} f_{ij} = \sum_{i\in A,\ j\in S} f_{ij}^+ \\ &= \sum_{i\in S,\ j\in B} f_{ij} = \sum_{i\in S,\ j\in B} f_{ij}^+.\end{aligned} \tag{33}$$

One can obtain another expression for the reaction rate ν_R as the total reactive current through an arbitrary cut. A *cut* in a network $G(S,E)$ is a partition of the nodes in S into two disjoints subsets that are joint by at least one edge in E. The set of edges whose endpoints are in different subsets of the partition is referred to as the cut-set. Here we will focus on A-B-cuts that are such that A and B are on different sides of the cut-set. Any A-B-cut leads to the decomposition $S = S_A \cup S_B$ such that $S_A \supseteq A$ and $S_B \supseteq B$ (see Fig. 6).

Theorem 25. *The transition rate ν_R is given by*

$$\nu_R = \sum_{i\in S_A}\sum_{j\in S_B} F_{i,j}, \tag{34}$$

where $F_{i,j} := f_{ij}-f_{ji}$ and $S_A\cup S_B$ is an arbitrary AB-cut.

Proof. We will use the fact that for any subset $S'\subset S$,

$$\sum_{i\in S', j\in S'} F_{i,j} = 0 \tag{35}$$

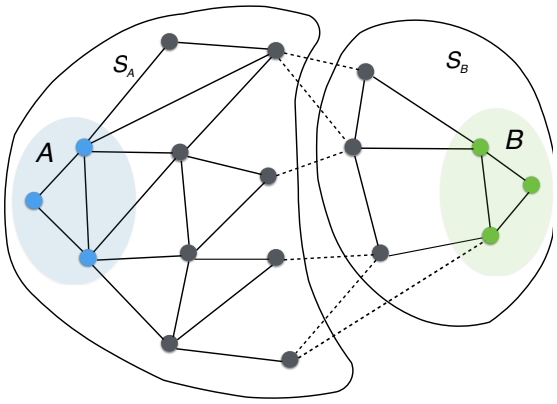


FIGURE 6. Illustration for the concept of an A-B-cut. The edges of the cut-set are shown with dashed lines.

because for every term $F_{i,j} = f_{ij} - f_{ji}$ in this sum there is a term $-F_{i,j} = f_{ji} - f_{ij}$. We have:

$$\sum_{i\in S_A, j\in S_B} F_{i,j} = \sum_{\substack{i\in A\cup(S_A\setminus A)\\ j\in(S\setminus S_A)}} F_{i,j}$$

$$= \sum_{\substack{i\in A\\ j\in S}} F_{i,j} + \sum_{\substack{i\in S_A\setminus A\\ j\in S}} F_{i,j} - \sum_{\substack{i\in S_A\\ j\in S_A}} F_{i,j} \tag{36}$$

$$= \nu_{AB} + 0 - 0 = \nu_{AB}. \tag{37}$$

The second sum in (36) is zero by current conservation, while the third sum is zero by (35). □

5.8. **Reaction pathways.** The effective current $f^+ = (f^+_{ij})_{i,j\in S}$ defined by Eq. (32) induces a directed graph with the set of states S. In other words, we connect states i and j by a directed edge $(i \to j)$ if and only if $f^+_{ij} > 0$. We denote this graph by $G\{f^+\}$.

Definition 21. *A reaction pathway $w = (i_0, i_1, \dots, i_n)$ is a simple (containing no loops) directed path in the graph $G\{f^+\}$ such that*

$$i_0 \in A,\ i_n \in B,\ i_k \in (A\cup B)^c,\ 1 \le k \le n-1.$$

5.9. **Simplifications for time-reversible Markov chains.** The case where the Markov chain is time reversible, i.e., $\hat{L} = L$ which is equivalent to the statement that L and π are in detailed balance, i.e.,

$$\pi_i L_{ij} = \pi_j L_{ji}$$

is worth of special consideration. Many interesting systems possess this property, and the formulas for the backward committor, the reactive current and for the transition rate can be given in terms of the forward committtor.

Exercise (1) Show that the forward and backward committor are related via

$$q_i^- = 1 - q_i^+, \quad i \in S.$$

Hence we can simplify the notations: denote the forward commuter by $q = (q_i)_{i\in S}$. Then the backward commuter is merely $1 - q$.

(2) Show that the reactive current $F_{ij} := f_{ij} - f_{ji}$ is given by

$$F_{ij} = \pi_i L_{ij}(q_j - q_i).$$

(3) Starting from the expression for the transition rate from A to B (the reaction rate) $\nu_R = \sum_{i\in A, j\in S} F_{ij}$, show that it can be rewritten as

$$\nu_R = \frac{1}{2}\sum_{i,j\in S} \pi_i L_{ij}(q_j - q_i)^2. \tag{38}$$

Besides the transition rate ν_R, one can consider the rates $k_{A,B}$ and $k_{B,A}$ defined as the inverse of the average times the last set hit by the trajectory was A or B, respectively. These rates are given by

$$k_{A,B} = \nu_R/\rho_A, \qquad k_{B,A} = \nu_R/\rho_B, \tag{39}$$

where

$$\rho_A = \sum_{i\in S} \pi_i(1 - q_i), \qquad \rho_B = \sum_{i\in S} \pi_i q_i \qquad (\rho_A + \rho_B = 1) \tag{40}$$

are the proportions of time such that the trajectory last hit A or B, respectively.

The directed graph $G\{f^+\}$ induced by the effective current contains no directed cycles in the case of detailed balance because every its directed edge connects a state with a smaller value of the committor q with a state with a large value of the committor. As a result, the committor is strictly increasing along every directed path in the graph $G\{f^+\}$ (see Fig. 7).

We can use cuts to characterize the width of the transition tube carrying the current of reactive trajectories. A specific set of cuts is convenient for this purpose, namely the family of isocommittor cuts which are such that their cut-set C is given by

$$C(q^*) = \{(i,j) \mid q_i \le q^*, q_j > q^*\}, \qquad q^* \in [0,1). \tag{41}$$

Isocommittor cuts [8] are special because if $i \in C_L$ and $j \in C_R$, the reactive current between these nodes is nonnegative, $F_{ij} \ge 0$, which also mean that every reaction pathway (no-detour reactive trajectory) contains exactly one edge belonging to an isocommittor cut since the committor increases monotonically along these transition paths. Therefore, we can sort the edges in the isocommittor cut $C(q)$ according to the reactive current they carry, in descending order, and find the minimal number of edges $N(q)$ carrying at least $p\%$ of this current. By doing so for each value of the committor $0 \le q \le 1$ and for different

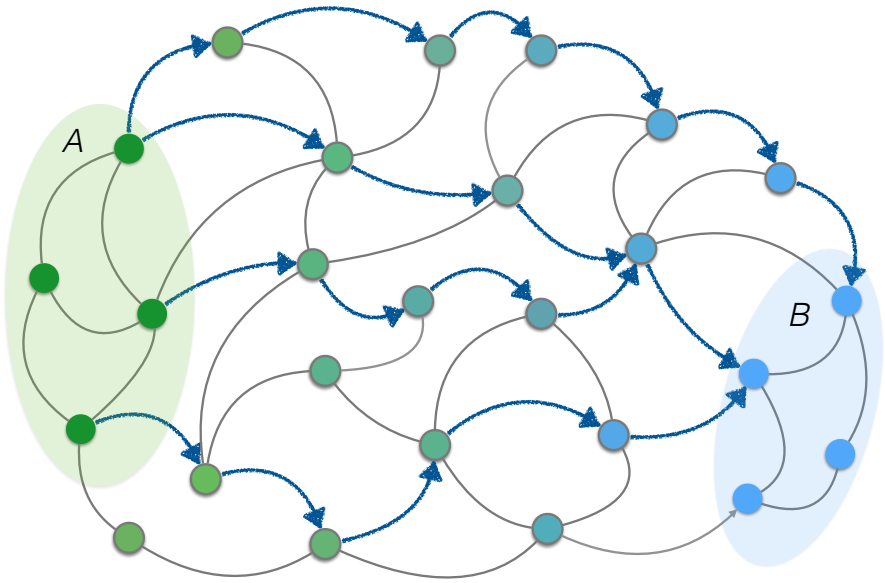


FIGURE 7. Examples of reaction pathways in the case of detailed balance are shown by blue arrows. The values of the committor are coded by color: green: $q = 0$, blue: $q = 1$. Note that the sequences of values of the commuter strictly increase along reaction pathways.

values of the percentage $p \in (0, 100)$, one can then analyze the geometry of the transition channel - how broad is it, how many sub-channels are they, etc.

Remark In the case of time-reversible Markov chains, the forward committor strictly increases along the edges of the graph $G(\{f^+\})$ (check this!). Therefore, the committor strictly increases along the reaction pathways. The reaction pathways were dubbed *no-detour reactive trajectories* in [8].

5.10. **Sampling reactive trajectories and no-detour reactive trajectories.** In this section, we assume that *the Markov chain under consideration is time-reversible* (i.e., π and L are in detailed balance). The probability current of reactive trajectories f_{ij} and effective current f^+_{ij} allow us to sample reactive trajectories and reaction pathways.

Recall that he probability current of reactive trajectories f_{ij} is the mean number of transitions performed by the reactive trajectories along the edge (i, j) per unit time, i.e., the transition rate for the reactive trajectories along the edge (i, j), we can replace the original generator matrix L with the generator matrix $\mathcal{F}$ whose off-diagonal entries are f_{ij} and the diagonal ones are defined so that the row sums of $\mathcal{F}$ are zeros.

Then one can convert the generator matrix $\mathcal{F}$ into the corresponding jump matrix $\Pi_{\mathcal{F}}$ according to Eq. (19) and generate a collection of reactive trajectories starting from states in A having outgoing edges.

One can do the same procedure but using the effective current f^+ instead of the probability current of reactive trajectories f. The detailed balance condition guaranties that these pathways are simple and the committer strictly increases along them.

Propositions justifying these instructions are found in [8].

Example 9 Consider the continuous-time Markov chain generated by a discretization of the overdamped Langevin dynamics

$$\frac{dx}{dt} = -\frac{\partial}{\partial x}V(x,y) + \sqrt{2T}\eta_x,$$
$$\frac{dy}{dt} = -\frac{\partial}{\partial y}V(x,y) + \sqrt{2T}\eta_y,$$

where η_x and η_y are independent white noises, on a 2D regular mesh with step h:

$$\{(y_i, x_j) \mid 1 \le i,j \le N,\ y_i = y_{\min} + (i-1)h,\ x_j = x_{\min} + (j-1)h\}.$$

We assume that the boundaries of the domain $[x_1, x_N] \times [y_1, y_N]$ are reflecting. From any non-boundary mesh point (state) (i,j) only transitions to its four nearest neighbors $(i+1,j)$ (North), $(i-1,j)$ (South), $(i,j+1)$ (East), and $(i,j-1)$ (West) are possible. The corresponding pairwise transition rates are

$$(i,j) \to (i+1,j): \quad L_N(i,j) = -\frac{1}{2h}\frac{\partial V}{\partial y}(i,j) + \frac{T}{h^2} \tag{42}$$

$$(i,j) \to (i-1,j): \quad L_S(i,j) = \frac{1}{2h}\frac{\partial V}{\partial y}(i,j) + \frac{T}{h^2} \tag{43}$$

$$(i,j) \to (i,j+1): \quad L_E(i,j) = -\frac{1}{2h}\frac{\partial V}{\partial x}(i,j) + \frac{T}{h^2} \tag{44}$$

$$(i,j) \to (i,j-1): \quad L_W(i,j) = \frac{1}{2h}\frac{\partial V}{\partial x}(i,j) + \frac{T}{h^2} \tag{45}$$

For the top and bottom boundaries L_N and L_S are modified as

$$L_N(N,j) = 0, \quad L_N(1,j) = \frac{2T}{h^2}, \tag{46}$$

$$L_S(1,j) = 0, \quad L_S(N,j) = \frac{2T}{h^2}, \tag{47}$$

while L_E and L_W are found by Eqs. (44)-(45). For the left and right boundaries L_E and L_W are modified as

$$L_E(i,N)=0,\quad L_E(j,1)=\frac{2T}{h^2}, \tag{48}$$

$$L_W(i,1)=0,\quad L_W(i,N)=\frac{2T}{h^2}, \tag{49}$$

while L_N and L_S are found by Eqs. (42)-(43). Therefore, the generator matrix L is 5-diagonal. Its diagonal entries are all equal to $-4T/h^2$. The forward and backward committors for this system are shown in Fig. 10 (a) and (b) respectively. A reactive trajectory superimposed with the probability distribution of reactive trajectories is shown in Fig. 10 (c). A collection of reaction pathways superimposed with the probability distribution of reactive trajectories is shown in Fig. 10 (d).

6. Metastability

In this Section, we will discuss the definition of metastability proposed by A. Bovier's group and their results regarding approximations for eigenvalues and eigenvectors [2, 3, 4].

Suppose we are considering a Markov Chain (discrete-time or continuous-time) with a finite set of states S. Let π be the invariant distribution. We assume that the chain is **time-reversible**. Let $M\subset S$ be a selected subset of states. Then the Markov chain is said to be metastable with respect to the set M if for any state $i\in M$ and for any state $j\in S\backslash M$, the probability that the process starting in at i will first reach some other state in M rather than come return to i is much less than the probability that the process starting at j will first reach any state in M rather than return to j. This definition of metastability can be written symbolically as follows.

Definition 22. *A Markov chain is metastable with respect to the subset of states M if*

$$\max_{i\in M}\mathbb{P}_i(\tau_{M\backslash i}<\tau_i)\ll\min_{j\in S\backslash M}\mathbb{P}_j(\tau_M<\tau_j). \tag{50}$$

An alternative formulation can be given in terms of mean hitting times. Recall that $E_i[\tau_A]$ is the the mean hitting time for the subset of states A for the process starting at state i.

Definition 23. *A Markov chain is metastable with respect to the subset of states M if*

$$\min_{i\in M}E_i[\tau_{M\backslash i}]\gg\max_{j\in S\backslash M}E_j[\tau_M]. \tag{51}$$

Definition 24. *If a Markov chain under consideration is metastable with respect to a subset of states $M\subset S$ then the subset of states M is called a metastable set.*

The main result of A. Bovier, M. Eckhoff, V. Gayrard, and M. Klein is the theorem giving sharp estimates for the eigenvalues and eigenvectors of the generator matrix L in the continuous-time case and of the matrix $P-I$ in the discrete-time case. Recall that the eigenvalues of L and $P-I$ are real and nonpositive.

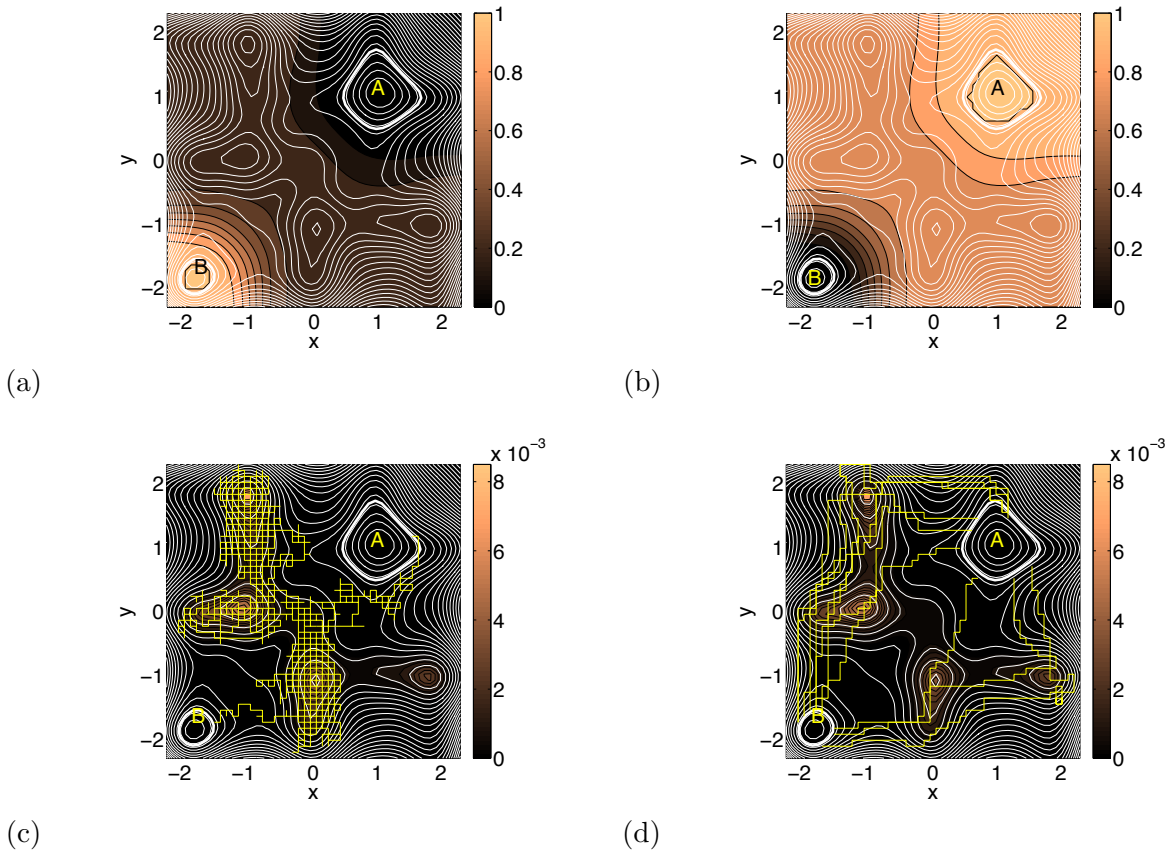


FIGURE 8. Example 9. Thin white curves show level sets of the 7-well potential. Thick white curves represent the boundaries of the sets A and B. (a): The forward committor. (b): The backward committor. (c): A reactive trajectory superimposed with the probability distribution of reactive trajectories. (d): A collection of reaction pathways superimposed with the probability distribution of reactive trajectories.

Theorem 26. *Assume that we can construct a sequence of metastable sets*

$$\begin{aligned} M_0 &= \{i_0\} \\ M_1 &= \{i_0, i_1\} \\ M_2 &= \{i_0, i_1, i_2\} \\ &\dots \\ M_p &= \{i_0, i_1, i_2, \dots, i_p\}. \end{aligned}$$

Denote by $\nu(A,B)$ the transition rate ν_R from A to B defined by Eq. (38), and by $q^{A,B}$ the forward committor with respect to the subsets of states A and B. Assume that one can find $\delta \ll 1$ such that for $0 \le k \le p$

$$\delta^2 \frac{\nu(i_k, M_k\backslash\{i_k\})}{\|q^{M_k\backslash\{i_k\},i_k}\|_{2,\pi}^2} \ge \max_{i_j \in M_k\backslash\{i_k\}} \frac{\nu(i_j, M_k\backslash\{i_j\})}{\|q^{M_k\backslash\{i_j\},i_j}\|_{2,\pi}^2}. \tag{52}$$

Then L has p eigenvalues $-\lambda_1, \dots, -\lambda_p$,

$$0 < \lambda_1 < \ldots < \lambda_p,$$

and

$$\lambda_k = \frac{\nu(i_k, M_{k-1})}{\sum_{j \in Valley(i_k)} \pi_j}(1 + O(\delta)) = \left(E_{i_k}[\tau_{M_{k-1}}]\right)^{-1}(1 + O(\delta)). \tag{53}$$

The corresponding eigenvector is given by

$$\phi_j^k = \frac{q_j^{M_{k-1},i_k}}{\|q^{M_{k-1},i_k}\|_{2,\pi}} + \sum_{l=1}^{k-1} O(\delta) \frac{q_j^{M_{l-1},i_k}}{\|q^{M_{l-1},i_k}\|_{2,\pi}}. \tag{54}$$

The norm $\|\cdot\|_{2,\pi}$ used in Theorem 26 is defined by

$$\|x\|_{2,\pi} = \sqrt{\sum_{i \in S} \pi_i x_i^2}.$$

To understand the statement of Theorem 26 we need the concept of *Valley*.

Definition 25. *Let $i \in M$ be a state in the metastable set M. The valley of i is the subset of states j in S such that given that the process starting at j has reached M, it is most likely that the process has reached the state i. I.e.,*

$$Valley(i) := \{j \in S \mid \mathbb{P}_j(\tau_i = \tau_M) = \max_{k \in M} \mathbb{P}_j(\tau_k = \tau_M)\}. \tag{55}$$

The definitions of the metastable set and the valley are illustrated in Fig. 9.
Theorem 26 says the following.

- Each eigenvalue $-\lambda_k$ corresponds to the escape process from $Valley(i_k)$ to M_{k-1}.
- The quantity
$$\frac{\nu(i_k, M_k\backslash\{i_k\})}{\|q^{M_k\backslash\{i_k\},i_k}\|_{2,\pi}^2}$$
in Eq. (52) is approximately the escape rate from i_k to $M_k\backslash\{i_k\} \equiv M_{k-1}$. Therefore, the condition given by Eq. (52) says that the expected time to reach M_{k-1} for the process starts at i_k is much less (at least by the factor δ^2) than the expected time to reach $M_k\backslash\{i_j\}$ starting from i_j for any $i_j \in M_{k-1}$.
- The number δ in this theorem is a small parameter. If the Markov chain represents an energy landscape where the pairwise transition rates are of the form
$$L_{ij} = \frac{b_{ij}}{b_i} \exp\left(-\frac{V_{ij} - V_i}{T}\right), \tag{56}$$

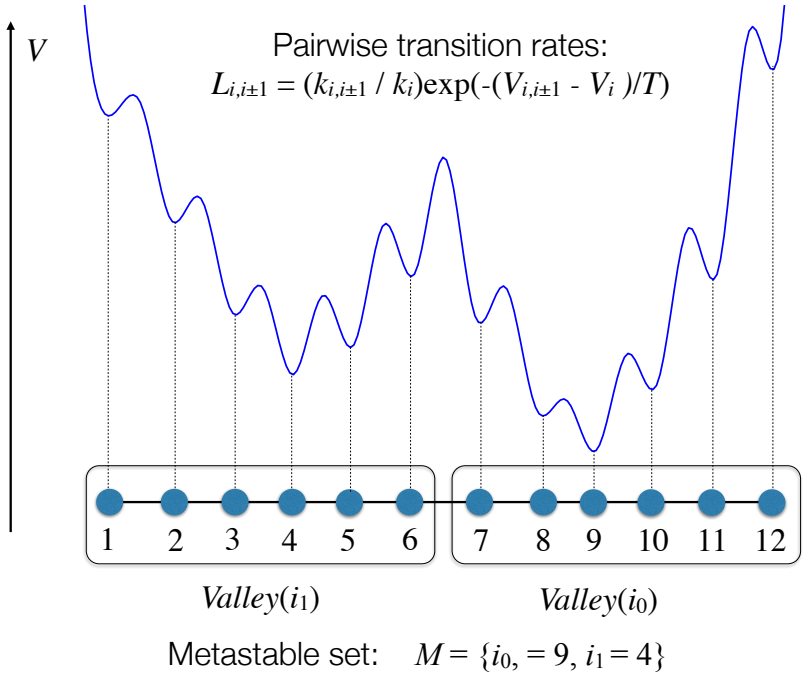


FIGURE 9. An illustration for the definitions of the metastable set and the valley on the example of a chain-of-states network with pairwise transition rates of the form $L_{i,i\pm1} = (k_{i,i\pm1}/k_i)\exp(-(V_{i,i\pm1} - V_i)/T)$, where T is the temperature.

where T is the temperature (measured in reduced units where $k_B = 1$), $\delta \to 0$ as $T \to 0$. In Eq. (56), V_i is the potential energy at the local minimum i, V_{ij} is the potential energy at the saddle separating i from the adjacent local minimum j, the factors b_i and b_{ij} are obtained using certain geometric characteristics of minimum i and saddle ij respectively.

The mean hitting times of sets M_{k-1} starting from states i_k are approximated by

$$\lambda_k \approx \left(E_{i_k}[\tau_{M_{k-1}}]\right)^{-1} \approx \frac{b_{p_k^* q_k^*}}{b_{i_k}} e^{-(V_{p^*q^*} - V_{i_k})/T}, \tag{57}$$

where $V_{p^*q^*}$ is the lowest possible highest potential barrier separating i_k and the set M_{k-1}, and $b_{p_k^* q_k^*}$ and b_{i_k} are the pre-exponential factors present in Eq. (56) corresponding to the edge $(p_k^* q_k^*)$ and the state i_k respectively. Eq. (57) was originally presented in [6] (see Eqs. (13)–(19)). A detailed proof of this fact is found in [7].

Example 10 Consider the "chain-of-states" network shown in Fig. 9 with pairwise transition rates of the form $L_{ij} = (b_{ij}/b_i)\exp(-(V_{ij}-V_i)/T)$, where T is the temperature. In this example, $M_0 = \{i_0\}$ and $M_i = \{i_0, i_1\}$. Assume that the temperature is small. The eigenvalue corresponding to the escape process from the $Valley(i_1)$ is approximated by

$$\lambda_1 \approx (E_{i_1}[\tau_{i_0}])^{-1} \approx \frac{b_{67}}{b_4}\exp\left(-\frac{V_{67}-V_4}{T}\right).$$

The corresponding eigenvector is approximated by the indicator function of $Valley(i_1)$, i.e.,

$$\phi_j^1 \approx \begin{cases} 1, & j \in Valley(i_1), \\ 0, & j \notin Valley(i_1). \end{cases}$$

7. More on spectral analysis: eigencurrents

The next three sections are taken from [9].

In this Section, we discuss what can we learn from the spectral decomposition of the generator matrix describing the dynamics of a stochastic network.

7.1. **The eigenstructure of networks with detailed balance.** In this Section, we provide some background and introduce some notations. Let $G(S, E, L)$ be a network, where S and E are its sets of states and edges respectively. We assume that the number of states is finite and denote it by N. The dynamics of this network is described by the generator matrix $L = \{L_{ij}\}_{i,j=1}^N$. If states i and j ($i \neq j$) are connected by an edge, then L_{ij} is the pairwise transition rate from i to j, otherwise $L_{ij} = 0$. The diagonal entries L_{ii} are defined so that the row sums of the matrix L are zeros. This fact implies that L has a zero eigenvalue $\lambda_0 = 0$ whose right eigenvector can be chosen to be $e := [1, 1, \ldots, 1]^\top$, i.e., $Le = 0$. The corresponding left eigenvector can be chosen to be the equilibrium probability distribution $\pi = [\pi_1, \pi_2, \ldots, \pi_N]$:

$$\pi L = 0, \quad \sum_{i=1}^N \pi_i = 1.$$

The generator matrices of networks representing energy landscapes possess the detailed balance property, i.e., $\pi_i L_{ij} = \pi_j L_{ji}$ which means that on average, there is the same numbers of transitions from i to j and from j to i per unit time. The detailed balance implies that the matrix L can be decomposed as

$$L = P^{-1}Q$$

where P is the diagonal matrix

$$P = \mathrm{diag}\{\pi_1, \pi_2, \ldots, \pi_N\},$$

and Q is symmetric. Hence L is similar to a symmetric matrix:

$$L_{sym} := P^{1/2}LP^{-1/2} = P^{-1/2}QP^{-1/2}. \tag{58}$$

Using Eq. (58) and that $L_{ii} = -\sum_{j\neq i} L_{ij}$ where $L_{ij} \geq 0$, one can show that eigenvalues of L are real and nonpositive. Furthermore, we assume that the network is connected. Hence L is irreducible and the zero eigenvalue has algebraic multiplicity one. We will denote the nonzero eigenvalues of L by $-\lambda_k$, $k = 1, 2, \ldots, N-1$, and order them so that

$$0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{N-1}.$$

The eigendecomposition of a generator matrix L leads to a nice representation of the time evolution of the probability distribution. The matrix L can be written as

$$L = \Phi\Lambda\Phi^\top P, \tag{59}$$

where $\Phi = [\phi^0, \phi^1, \ldots, \phi^{N-1}]$ is a matrix of right eigenvectors, normalized so that $P^{1/2}\Phi$ is orthogonal. Note that $P^{1/2}\Phi$ is the matrix of eigenvectors of L_{sym}. Therefore,

$$\|P^{1/2}\phi^k\|^2 = \sum_{j=1}^{N} \pi_j |\phi_j^k|^2 = 1, \tag{60}$$

$$\sum_{j=1}^{N} \pi_j \phi_j^k \phi_j^l = 0, \quad k \neq l, \tag{61}$$

and in particular, $\phi^0 = e$ and $P\phi^0 = \pi$.

The probability distribution evolves according to the Forward Kolmogorov (a. k. a. the Fokker-Planck) equation

$$\frac{dp}{dt} = pL, \quad p(0) = p_0,$$

where p_0 is the initial distribution. Using Eqs. (59)–(61) we get

$$p(t) = \sum_{k=0}^{N-1} c_k e^{-\lambda_k t} \left(P\phi^k\right)^\top, \text{ where } c_k = p_0\phi^k. \tag{62}$$

Note that $c_0 = p_0[1, \ldots, 1]^\top = \sum_{j=0}^{N}(p_0)_j = 1$. Eq. (62) shows that the k-th eigen-component of $p(t)$ remains significant only on the time interval $O(\lambda_k^{-1})$. Eventually, all eigen-components, except for the zeroth, decay. Hence $p(t) \to \pi$ as $t \to \infty$.

7.2. **Interpretation of eigenvalues and eigenvectors.** For $k > 0$, the left and right k-th eigenvectors of L, $[P\phi^k]^\top$ and ϕ^k respectively, can be understood from a recipe for preparing the initial probability distribution so that only the coefficients c_0 and c_k in Eq. (62) are nonzero. Imagine $n \gg 1$ particles distributed in the stochastic network according to the equilibrium distribution π. Since $(\phi^0)^\top P\phi^k = \sum_{j=1}^{N} \pi_j \phi_j^k = 0$ for any $k > 0$, the set of states S can be divided into two parts:

$$S_+^k := \{i \in S \ : \ \phi_i^k \geq 0\} \quad \text{and}$$
$$S_-^k := \{i \in S \ : \ \phi_i^k < 0\}. \tag{63}$$

In order to create a component of the initial distribution parallel to the left eigenvector $[P\phi^k]^\top$, we pick some α satisfying $\alpha\phi_j^k \leq 1$ for all $j \in S_-^k$, remove $\alpha n \pi_j |\phi_j^k|$ particles from

each state $j \in S_-^k$ and distribute them in S_+^k so that each state $j \in S_+^k$ gets $\alpha n \pi_j \phi_j^k$ particles. The resulting distribution p_0 is $\pi + \alpha[P\phi^k]^\top$. Therefore, the left eigenvector $\alpha[P\phi^k]^\top$ is a perturbation of the equilibrium distribution decaying uniformly across the network with the rate given by the corresponding eigenvalue λ_k. (The keyword here is "uniformly".) The corresponding right eigenvector $\alpha\phi^k$ shows for each state $j \in S$, by which proportion of π_j state j is over- or underpopulated in the perturbed distribution $\pi + \alpha[P\phi^k]^\top$. Therefore, ϕ^k is, in essence, a fuzzy signed indicator function of the perturbation $[P\phi^k]^\top$.

7.3. **Eigencurrents.** The importance of probability currents for the quantitative description of transition processes in the system was emphasized in works of J. Kurchan (see e.g. Six out of equilibrium lectures). For example, the reactive current is one of the key concepts of the Transition Path Theory [14, 8]. In the context of spectral analysis, E. Vanden-Eijnden proposed to consider the eigencurrent [8]. While eigenvectors determine the perturbations to the equilibrium distribution decaying with the rates given by the corresponding eigenvalues, eigencurrents give a quantitative description of the escape process from these perturbed distributions.

Eigencurrents are defined as follows. The time derivative of the i-th component of the probability distribution $p(t)$ is

$$\frac{dp_i}{dt} = \sum_{j=1}^{N} L_{ji} p_j = \sum_{j \neq i} (L_{ji} p_j - L_{ij} p_i). \tag{64}$$

Plugging in expressions for p_i and p_j from Eq. (62) into Eq. (64) and using the detailed balance property $\pi_i L_{ij} = \pi_j L_{ji}$ we obtain

$$\frac{dp_i}{dt} = \sum_{k=0}^{N-1} c_k e^{-\lambda_k t} \sum_{j \neq i} \pi_i L_{ij} [\phi_j^k - \phi_i^k]. \tag{65}$$

The collection of numbers

$$F_{ij}^k := \pi_i L_{ij} e^{-\lambda_k t} [\phi_i^k - \phi_j^k] \tag{66}$$

is called the eigencurrent associated with the k-th eigenpair. (Here we have switched the sign and incorporated the factor $e^{-\lambda_k t}$ into the definition in comparison with the one in Ref. [8] in order to make its physical sense more transparent.) In terms of the eigencurrent F_{ij}^k, Eq. (65) can be rewritten as

$$\frac{dp_i}{dt} = -\sum_{k=0}^{N-1} c_k \sum_{j \neq i} F_{ij}^k. \tag{67}$$

Hence, the eigencurrent F_{ij}^k is the net probability current of the k-th perturbation $P\phi^k$ along the edge (i, j) per unit time. In other words, if the system is originally distributed according to $p_0 = \pi + \alpha P \phi_k$ then the current αF_{ij}^k gives the difference of the average numbers of transitions from i to j and from j to i per unit time.

The eigencurrent F_{ij}^k can be compared to the reactive current F_{ij} in Ref. [8] (which is the same as the quantity $f_{ij}^{AB} - f_{ji}^{AB}$ in Ref. [14]). The reactive current F_{ij} is conserved at every node of the network [14] except for the specially designated subsets of source states A and sink states B. Contrary to it, the eigencurrent is either emitted or absorbed in all states i where $\phi_i^k \neq 0$. Indeed, for any $i \in S$ we have

$$\begin{aligned}\sum_{j\neq i} F_{ij}^k =& \pi_i e^{-\lambda_k t}\left[\phi_i^k \sum_{j\neq i} L_{ij} - \sum_{j\neq i} L_{ij}\phi_j^k\right] \\ =& \pi_i e^{-\lambda_k t}\left[-\sum_{j=1}^{N} L_{ij}\phi_j^k\right] = e^{-\lambda_k t}\lambda_k \pi_i \phi_i^k. \end{aligned} \tag{68}$$

Therefore, every state i emits or absorbs (depending on the sign of ϕ_i^k) $e^{-\lambda_k t}\lambda_k \pi_i |\phi_i^k|$ units of the eigencurrent F_{ij}^k per unit time.

Let's partition the set of states S into S_+^k and S_-^k (see Eq. (63)). The corresponding cut-set (a. k. a. cut) consists of all edges (i, j) where $\phi_i^k \geq 0$ and $\phi_j^k < 0$. We will call this cut the emission-absorption cut as it separates the states where the eigencurrent F_{ij}^k is not absorbed from those where it is absorbed. It can be compared to the isocommittor cut [8] corresponding to the committor value $q = 0.5$.

Now we will show that for every fixed time t, the eigencurrent over the emission-absorption cut is maximal among all possible cuts of the network, and it is equal to the total eigencurrent emitted by the states S_+^k per unit time at time t, i.e.,

$$\begin{aligned}&\max_{S',S'':\ S=S'\dot\cup S''} \sum_{i\in S', j\in S''} F_{ij}^k \\ &= \sum_{i\in S_+^k, j\in S_-^k} F_{ij}^k = e^{-\lambda_k t}\lambda_k \sum_{i\in S_+^k} \pi \phi_i^k \end{aligned} \tag{69}$$

(The symbol $\dot\cup$ denotes the disjoint union.) Since Eq. (66) implies that $F_{ij}^k = -F_{ji}^k$, for any subset $S' \subset S$ we have

$$\sum_{i\in S', j\in S'} F_{ij}^k = 0.$$

Therefore, the eigencurrent over the cut (S', S'') is

$$\begin{aligned}\sum_{i\in S',\ j\in S''} F_{ij}^k =& \sum_{i\in S',\ j\in S} F_{ij}^k - \sum_{i\in S',\ j\in S'} F_{ij}^k \\ =& e^{-\lambda_k t}\lambda_k \sum_{i\in S'} \pi_i \phi_i^k, \end{aligned}$$

i.e., it is the total eigencurrent emitted in S' per unit time. The maximum of the last sum is achieved if $S' = S_+^k$, i.e., if S' consists of all non-absorbing states.

The cut-set of the emission-absorption cut is the true transition state of the relaxation process from the perturbed distribution $\pi + \alpha[P\phi^k]^\top$.

8. The spectral analysis versus TPT

In this Section, we will summarize the similarities and differences between the spectral analysis and TPT (Transition Path Theory).

The basic steps of the analysis of a transition process taking place in the stochastic network $G(S, E, L)$ by means of TPT are the following. We assume detailed balance for simplicity.

(1) Pick two disjoint subsets of states: a source set $A \subset S$ and a sink set $B \subset S$.

(2) Solve the committor equation

$$\sum_{j\in S} L_{ij}q_j = 0,\ i \in S\backslash(A \cup B), \quad q(A) = 0, \quad q(B) = 1. \tag{70}$$

For each state i the value of the committor q_i is the probability that the random walk starting at i will reach first B rather than A.

(3) Calculate the reactive current

$$F^R_{ij} := \pi_i L_{ij}(q_j - q_i)$$

and analyze it. For example, one can consider its distribution in the isocommittor cuts and visualize the reactive tube with their aid. (For a given $q \in [0, 1)$ the isocommittor cut [8] $C(q)$ is the collection of edges (i, j) such that $q_i \le q$ and $q_j > q$.)

(4) Calculate the transition rate ν_R, i.e., the average number of transitions from A to B per unit time, e.g. by

$$\nu_R = \sum_{(i,j)\in C(q)} F^R_{ij},$$

where $C(q)$ is an arbitrary isocommittor cut. Also calculate the rates $k_{A,B}$ and $k_{B,A}$ which are the inverse average times of going back to B after hitting A and going back to A after hitting B respectively. They are given by

$$k_{A,B} = \frac{\nu_R}{\sum_{i\in S}\pi_i(1 - q_i)}, \quad k_{A,B} = \frac{\nu_R}{\sum_{i\in S}\pi_i q_i}.$$

In TPT, the probability distribution in the network is assumed to be equilibrium, i.e., π. The transition process from A to B is stationary. The committor, the reactive current, and the transition rates are time-independent. Contrary to this, the eigenpair (λ_k, ϕ^k) describes the time-dependent relaxation process starting from the non-equilibrium distribution $\pi + \alpha[P\phi^k]^\top$, where the perturbation $\alpha[P\phi^k]^\top$ decays uniformly throughout the network with the rate λ_k.

Nevertheless, it is instructive to compare the right eigenvector ϕ^k to the committor, the eigencurrent

$$F^k_{ij} = \pi_i L_{ij}(\phi^k_j - \phi^k_i)e^{-\lambda_k t}$$

to the reactive current F^R_{ij}, and the transition rate $k_{A,B}$ to λ_k. We will do it on the example of the LJ_{38} network.

The committor and the right eigenvector play similar roles in the definitions of the corresponding currents. The net average numbers of transitions per unit time along the edge (i,j) done by reactive trajectories and during the relaxation process are proportional to $\pi_i L_{ij}(q_j - q_i)$ and $\pi_i L_{ij}(\phi^k_j - \phi^k_i)$ respectively. However, there are important differences between the right eigenvector and the committor. While the committor indicates the probability to reach first B rather than A starting from the given state, the right eigenvector indicates how the given state is over- or underpopulated relative to the equilibrium distribution. The committor takes values in the interval $[0,1]$, while the range of values of the components of the right eigenvector $\phi^{(\mathrm{ICO})}$, normalized as described in Section 7.1, is temperature dependent. Some components acquire values much larger than 1 or much less than -1.

Both the reactive current F^R_{ij} and the eigencurrent F^k_{ij} describe the net probability flow for the corresponding processes. The reactive current is time-independent, while the eigencurrent uniformly decays with time at the rate λ_k. The reactive current is emitted by the source states A, absorbed by the sink states B and conserved at all other states. There is no reactive current between any two source states, and there is no reactive current between any two sink states. Contrary to this, the eigencurrent is emitted at all states where $\phi^k > 0$, absorbed at all states where $\phi^k < 0$, and there is a nonzero eigencurrent along any edge (i,j) as long as $\phi^k_i \neq \phi^k_j$. The total flux of the reactive current is the same through any cut of the network separating the sets A and B. The total flux of the eigencurrent is maximal through the emission-absorption cut, which is the cut separating the states with $\phi^k_j \geq 0$ and $\phi^k_j < 0$. Note if $\phi^k_j = 0$ at some state j, then the emission-absorption cut is not the only cut separating the states with $\phi^k > 0$ and $\phi^k < 0$. In this case, the flux of the eigencurrent is maximal through any cut separating the states with $\phi^k > 0$ and $\phi^k < 0$.

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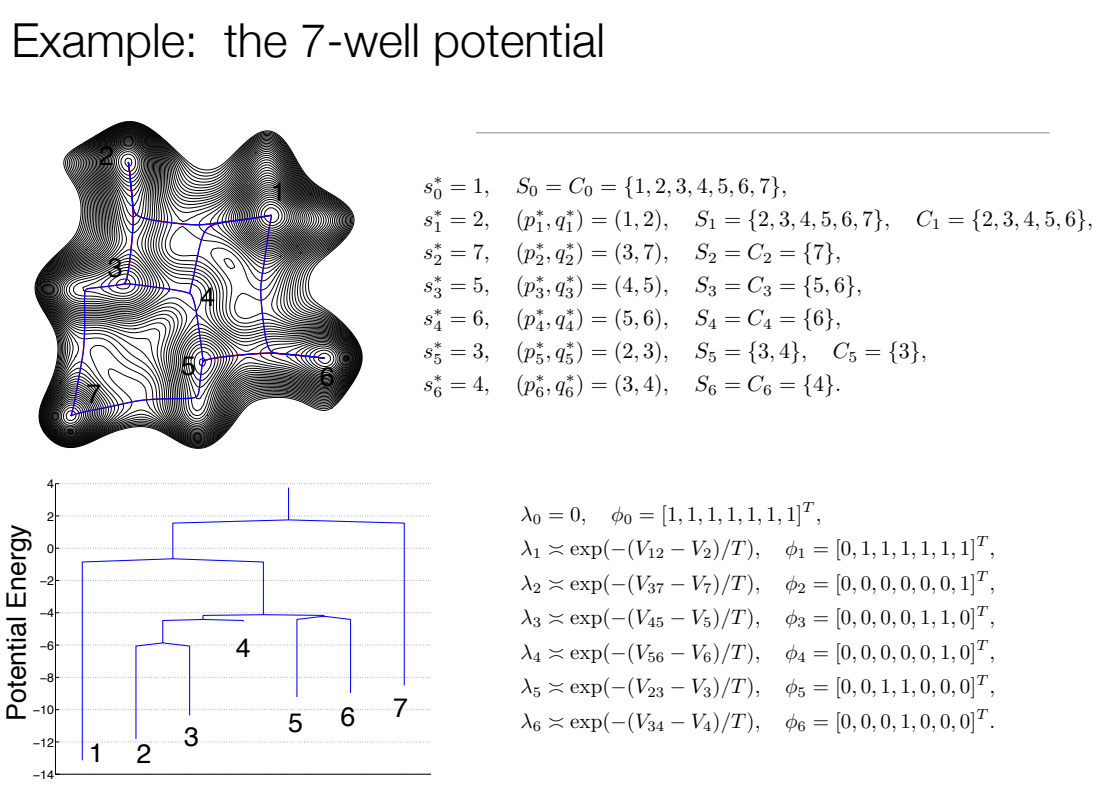

FIGURE 10. An example of 7-well potential.

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