MARKOV CHAINS

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Contents

These notes are largely based on the book "Markov Chains" by J. R. Norris [1]. These Cambridge University notes are also based on the same book.

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

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

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)

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

(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 $i_1, \dots, i_{n-1}$ such that

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

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*

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

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 $\{1, 2, \dots\} =: C_1$ 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 [8]. 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 [7]. 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:

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

1.3. Hitting times and absorption probabilities.

Definition 4. *Let $(X_n)_{n\ge0}$ be a Markov chain with transition matrix P. The hitting time of a subset $A \subset S$ is the random variable $\tau_A : \Omega \to \{0,1,2,\dots\} \cup \{\infty\}$ given by*

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

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

Definition 5.

- *The probability that $(X_n)_{n\ge0}$ ever hits A starting from state i is*

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

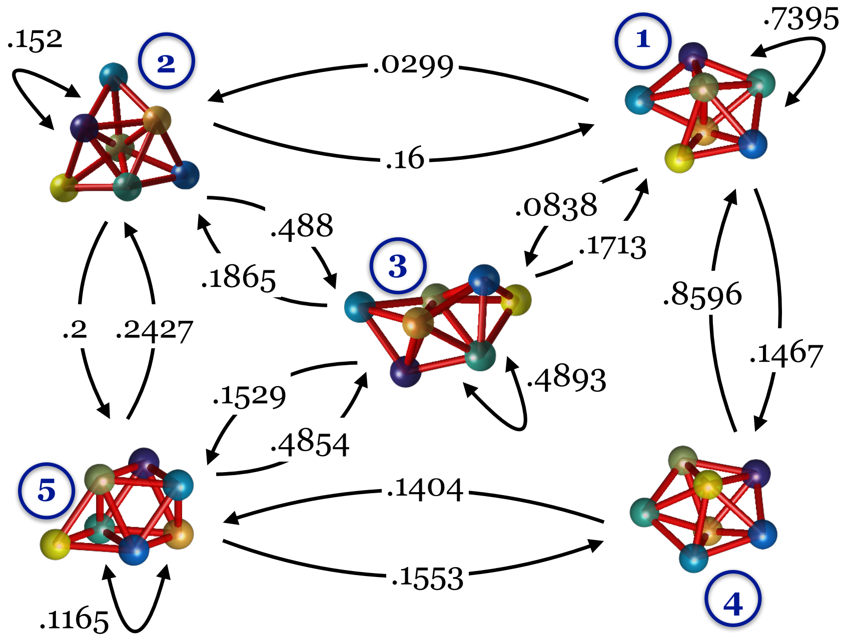

FIGURE 1. A jump chain for 7 particles interacting according to a sticky potential obtained from Fig. 6 in [7].

- *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 non-negative 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. *Assume that $h_i^A > 0$ for all $i \in (S \backslash A)$. The vector of mean hitting times $k^A = \{k_i^A \mid i \in S\}$ is the minimal non-negative 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 the desired equation:

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

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:

$$\begin{aligned} y_i =& \mathbb{P}_i(\tau^A \geq 1) + \mathbb{P}_i(\tau^A \geq 2) + \ldots \mathbb{P}_i(\tau^A \geq n) + \sum_{j_1 \notin A} \cdots \sum_{j_n \notin A} p_{ij_1} p_{j_1 j_2} \ldots p_{j_{n-1} j_n} y_{j_n} \\ =& \mathbb{P}_i(\tau^A = 1) + 2\mathbb{P}_i(\tau^A = 2) + \ldots + n\mathbb{P}_i(\tau^A \geq n) + \sum_{j_1 \notin A} \cdots \sum_{j_n \notin A} p_{ij_1} p_{j_1 j_2} \ldots p_{j_{n-1} j_n} y_{j_n}. \end{aligned}$$

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

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

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 shown in Fig. 2(b). Let P_i be the probability for the particle to disappear

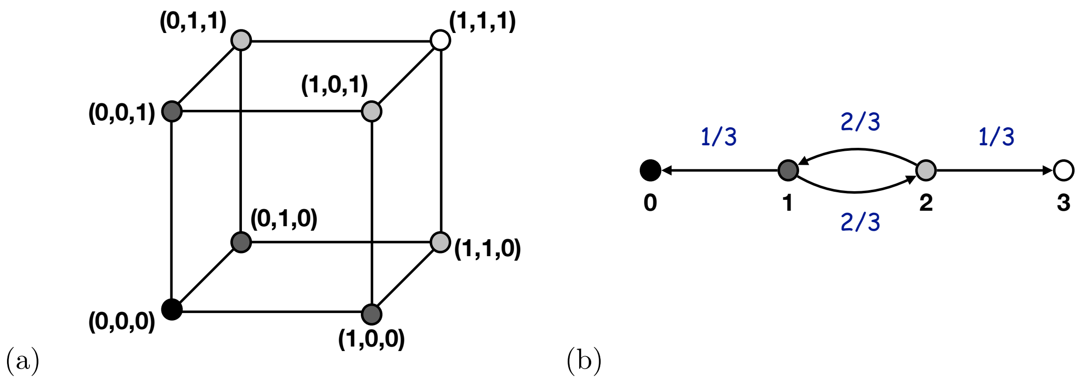

FIGURE 2. Illustration for Example 5

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 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

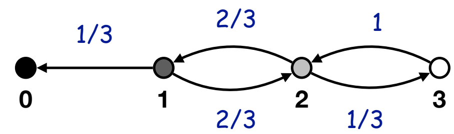

FIGURE 3. Illustration for Example 6

have:

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

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 $\{0, 1, 2, \dots\}$, 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 $S = \{0, 1, 2, \dots\}$ 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

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

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,

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

Then

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

Hence

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

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 $i\ge 1$.

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:

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

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 $p\le 1/2$, then $\frac{1-p}{p}\ge 1$, 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 $p\le 1/2$, and $P_1=\frac{1-p}{p}$ if $p>1/2$.

1.5. Recurrence and transience.

Definition 6. *Let $(X_n)_{n\ge 0}$ 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*

$$T_i(\omega)=\inf\{n\ge 1 \mid X_n(\omega)=i\},\quad \text{where} \quad \inf\emptyset=\infty.$$

- *The rth passage time to state i is the random variable $T_i^{(r)}$ defined inductively by*

$$T_i^{(0)}=0,\quad T_i^{(r+1)}=\inf\{n\ge T_i^{(r)}+1 \mid X_n(\omega)=i\},\quad r=0,1,2,\dots.$$

- *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

$$E_i[V_i] = E_i\left[\sum_{n=0}^{\infty} 1_{\{X_n=i\}}\right] = \sum_{n=0}^{\infty} E\left[1_{\{X_n=i\}}|X_0=i\right]$$

$$= \sum_{n=0}^{\infty} \mathbb{P}_i(X_n=i) = \sum_{n=0}^{\infty} p_{ii}^{(n)}. \tag{8}$$

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

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

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

(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 $i\in S$*

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

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

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

□

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*

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

In particular,

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

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 $e = [1, \dots, 1]^\top$.

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 $m_1 + \dots + m_r = N - 1$, 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

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

(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 backward. 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.

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

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

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):

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

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

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 $\pi\hat{P} = \pi$:

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

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

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

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

□

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

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 $\mathsf{Markov}(\lambda, \mathsf{P})$ 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 $\mathsf{Markov}(\lambda, \mathsf{P})$.*

Theorem 12. *Let P be an irreducible stochastic matrix and let λ be a distribution. Suppose that $(X_n)_{n\geq 0}$ is $\mathsf{Markov}(\lambda, \mathsf{P})$. 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. Transition Path Theory

The Transition Path Theory (TPT) was introduced by W. E and E. Vanden-Eijnden in 2006 [5, 6] 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 mathematical framework for describing transitions between two subsets of interest often denoted by A and B. 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) [9] 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 [4].

The key difference in the works by A. Bovier on metastability [2] and the TPT is that the TPT does not assume that the MJP in-hand is time-reversible, while Bovier considers only reversible Markov chains [2].

In these lecture notes, we adapt TPT for discrete-time Markov chains. Let us recall that the generator L for diffusion processes evolving according to SDEs was defined by the limit

$$Lf := \lim_{t\to 0} \frac{P_t f - f}{t},$$

where P is the transfer operator. The analog of the transfer operator in the context of discrete-time Markov chains is the stochastic matrix P. The time is discrete, hence the minimal time advancement is 1. Therefore, the generator for discrete-time Markov chains is the matrix L defined by

$$L := P - I, \tag{11}$$

where I is the identity matrix. Note that the off-diagonal entries of L and P match. Therefore, the condition for the detailed balance can be rewritten in terms of L as

$$\pi_i L_{ij} = \pi_j L_{ji}, \quad \text{or, in matrix form} \quad \Pi L = (\Pi L)^\top,$$

where $\Pi := \mathsf{diag}\{\pi_1, \pi_2, \ldots, \pi_{|S|}\}$. Furthermore, the generator of the time-reversal of a chain with generator L is found from

$$\pi_i L_{ij} = \pi_j \hat{L}_{ji}, \quad \text{or, in matrix form} \quad \hat{L} = \Pi L \Pi^{-1}.$$

3.1. **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 and 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 $(\hat{X}_t)_{t \in \mathbb{Z}_+}$, $\hat{X}_t = X_{N-t}$ where N 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

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

3.2. **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., $(X_t)_{t \in \mathbb{Z}_+}$ 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

$$t_n^A < t_n^B < t_{n+1}^A \quad n \in \mathbb{N},$$
$$X(t_n^A) = x_n^A \in A, \quad X(t_n^B) = x_n^B \in B,$$
$$\text{for any} \;\; t_n^A < t < t_n^B \;\; X(t) \in (A \cup B)^c.$$

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 $\{t_n^A + 1, \ldots, t_n^B - 1\}$ are called *reactive times*. The union of the reactive times is denoted by R:

$$R := \bigcup_{n \in \mathbb{Z}} \{t_n^A + 1, \ldots, t_n^B - 1\}.$$

Definition 14. *The ordered sequence*

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

consisting of successive states of the Markov chain $(X_k)_{k\in\mathbb{Z}}$ *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. 4.

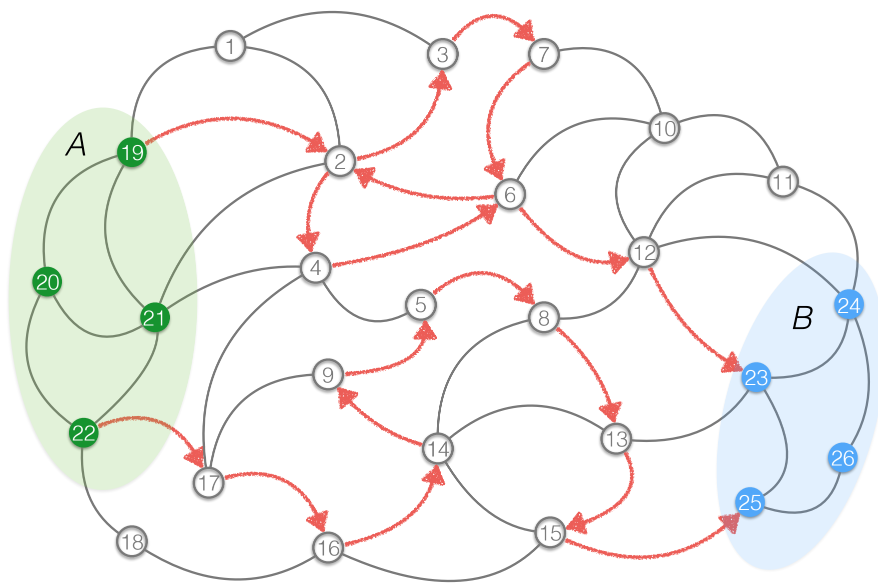

FIGURE 4. Two examples of reactive trajectories are shown in red. Reactive trajectory 1: [19, 2, 3, 7, 6, 2, 4, 6, 12, 23]. Reactive trajectory 2: [22, 17, 16, 14, 9, 5, 8, 13, 15, 25].

3.3. The forward and backward committors.

Definition 15. *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 $(\hat{X}_t)_{t\in\mathbb{Z}}$ is the time-reversed process for $(X_t)_{t\in\mathbb{Z}}$, i.e., $\hat{X}_t = X_{-t}$, $t \in \mathbb{Z}$.

The forward and backward committors satisfy the following equations:

$$\begin{cases} \sum_{j\in S} L_{ij} q_j^+ = 0, & i \in (A\cup B)^c, \\ q_i^+ = 0, & i \in A, \\ q_i^+ = 1, & i \in B, \end{cases} \tag{12}$$

and

$$\begin{cases} \sum_{j\in S} \hat{L}_{ij} q_j^- = 0, & i \in (A\cup B)^c, \\ q_i^- = 1, & i \in A, \\ q_i^- = 0, & i \in B, \end{cases} \tag{13}$$

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

Eq. (12) 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. (12) 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. (13).

3.4. **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

$$m_i^R = \pi_i q_i^- q_i^+. \tag{14}$$

In [9], 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.,

$$Z_R = \mathbb{P}(t \in \text{reacive time}).$$

3.5. **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

$$f_{ij} = \begin{cases} \pi_i q_i^- L_{ij} q_j^+, & i \neq j, \\ 0, & i = j. \end{cases} \tag{15}$$

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. (15) 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 13. *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:*

$$\sum_{j \in S} (f_{ij} - f_{ji}) = 0 \quad \text{for all} \quad i \in (A \cup B)^c. \tag{16}$$

Proof. Let $i \in (A \cup B)^c$. Plugging in Eq. (15) to Eq. (16) 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. (12) and (13) 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,

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

□

3.6. **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*:

$$f^+_{ij} := \max\{f_{ij} - f_{ji}, 0\}. \tag{17}$$

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.

3.7. **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.,

$$\begin{aligned}\nu_R &= \sum_{i\in A,\ j\in S} f_{ij} = \sum_{i\in A,\ j\in S} f^+_{ij}\\ &= \sum_{i\in S,\ j\in B} f_{ij} = \sum_{i\in S,\ j\in B} f^+_{ij}.\end{aligned} \tag{18}$$

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. 5).

Theorem 14. *The transition rate ν_R is given by*

$$\nu_R = \sum_{i\in S_A} \sum_{j\in S_B} F_{i,j}, \tag{19}$$

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 $S' \subset S$,

$$\sum_{i\in S', j\in S'} F_{i,j} = 0 \tag{20}$$

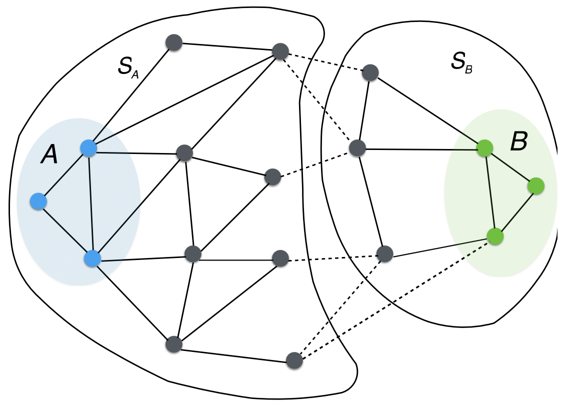

FIGURE 5. Illustration for the concept of an A-B-cut. The edges of the cut-set are shown with dashed lines.

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:

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

$$= \sum_{\substack{i\in A\\ j\in S}} F_{i,j} + \sum_{\substack{i\in S_A\setminus A\\ j\in S}} F_{i,j} - \sum_{\substack{i\in S_A\\ j\in S_A}} F_{i,j} \tag{21}$$

$$= \nu_{AB} + 0 - 0 = \nu_{AB}. \tag{22}$$

The second sum in (21) is zero by current conservation, while the third sum is zero by (20). □

3.8. **Reaction pathways.** The effective current $f^+ = (f^+_{ij})_{i,j\in S}$ defined by Eq. (17) 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 16. *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*

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

3.9. **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

$$\nu_R = \frac{1}{2}\sum_{i,j\in S} \pi_i L_{ij}(q_j - q_i)^2. \tag{23}$$

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

$$k_{A,B} = \nu_R/\rho_A, \qquad k_{B,A} = \nu_R/\rho_B, \tag{24}$$

where

$$\rho_A = \sum_{i\in S} \pi_i(1 - q_i), \qquad \rho_B = \sum_{i\in S} \pi_i q_i \qquad (\rho_A + \rho_B = 1) \tag{25}$$

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. 6).

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

$$C(q^*) = \{(i, j) \mid q_i \le q^*, q_j > q^*\}, \qquad q^* \in [0, 1). \tag{26}$$

Isocommittor cuts [4] 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

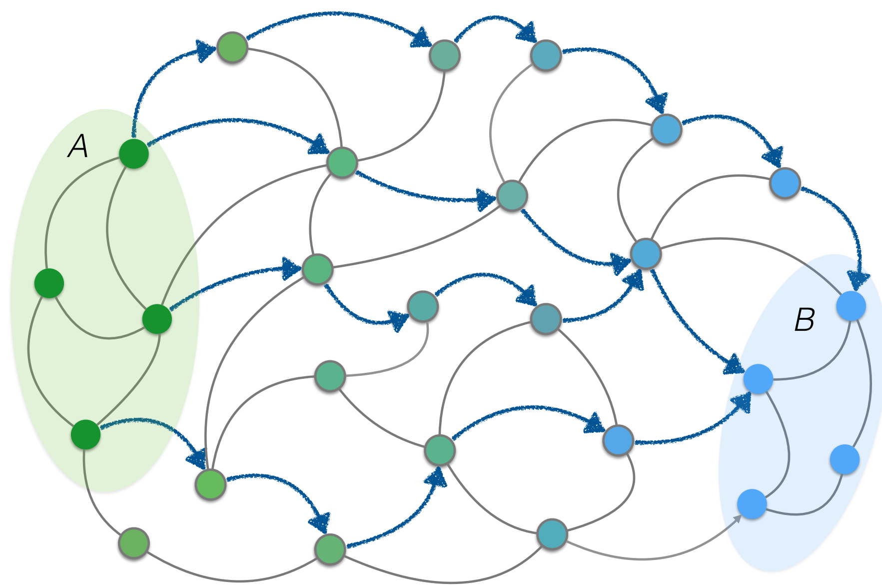

FIGURE 6. Examples of reaction pathways in the case of detailed balance are shown by blue arrows. The values of the committor are coded by color: green: $q = 0$, blue: $q = 1$. Note that the sequences of values of the commuter strictly increase along reaction pathways.

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 [4].

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