Part III

Sampling and Latent Estimation

10 Markov Chains

Piaget tried algebra and Freud tried diagrams; other psychologists used Markov Chains and matrices, but none came to much.
—Marvin Minsky

Markov chains famously play a key role in the Google PageRank algorithm for ranking websites. But Markov chains are important for machine learning in many other ways as well. One of their most significant applications is for sampling from otherwise-complicated probability distributions using *Markov chain Monte Carlo (MCMC)* methods. MCMC methods are fundamental to Bayesian statistics and inference, and many would say MCMC is the key tool that has made Bayesian inference possible. Another important application of Markov chains is for describing many time series models, including hidden Markov models, where the states of the Markov chain itself are not observed, and one can only observe some other quantity that is influenced by the state of the Markov chain. We discuss both of these applications (MCMC and hidden Markov models) in later chapters. In this chapter we develop the foundations of Markov chains that will be needed for those later applications.

10.1 Markov Chains

A Markov chain is a special kind of *stochastic process*. Stochastic processes are essentially just a sequence (or a continuous family) of random variables taking values in a common set. Stochastic processes, and especially Markov chains, are fundamental tools for modeling sequential data—data that follows a sequence or that depends on time.

10.1.1 Stochastic Processes

Definition 10.1.1. *A* stochastic process *is a family* $(X_t)_{t\in T}$ *of random variables on a common probability space* $(\Omega, \mathscr{F}, P)$ *taking values in a set* S *(usually a subset of* $\mathbb{R}^n$*). The index set* T *is often interpreted to be points in time, but that is not mathematically important. A stochastic process is discrete if* $T = \mathbb{N}$ *and continuous if either* $T = [0, \infty)$ *or* $T = (-\infty, \infty)$*. In this chapter, we assume that* $T = \mathbb{N}$ *unless otherwise stated. The set* S *is called the* state space *of the process.*

Example 10.1.2. A sequence $X_1, X_2, \ldots$ of i.i.d. random variables is an example of a stochastic process. When $X_i \sim \text{Bernoulli}(p)$, this is called a *Bernoulli process*.

Example 10.1.3. Imagine a person who starts at some point on the number line, and then flips a coin. If the coin shows heads, they move one step right, and otherwise they move one step left. They repeatedly flip the coin and move one step right with heads and one step left otherwise. Their position after t coin flips is a random variable $X_t = \sum_{i=1}^{t} Z_t$, where each Z_i is a random variable taking the value $+1$ if heads, and -1 if tails. The collection $(X_t)_{t\in\mathbb{N}}$ forms a stochastic process called a *simple random walk*.

More generally, for any sequence of i.i.d. random varables $(Z_t)_{t\in\mathbb{N}}$ taking values in $\mathbb{R}^n$, the sequence $X_t = \sum_{i=0}^{t} Z_i$ of sums is called a *random walk*.

Example 10.1.4. (Gambler's Ruin) A simple random walk corresponds to the wealth of a gambler who bets one dollar for each coin flip, provided he is allowed to have unlimited negative wealth and the person taking the other side of the bet has unlimited wealth. A more realistic model would account for the fact that if the gambler ever runs out of money ($X_k = 0$), then he is bankrupt and cannot bet any more, so $X_t = 0$ for all $t \geq k$. We call this a *simple random walk with an absorbing barrier*. Many casinos also have an upper limit on how much a person may win in one visit, in such cases there is also an absorbing upper barrier. If the limit is L, then once $X_k = L$ we always have $X_t = L$ for all $t \geq k$. A simple random walk with absorbing barriers is also a stochastic process.

Example 10.1.5. Given any stochastic process $(Z_i)_{i\in\mathbb{N}}$, the sequence of *nth moving averages* $\text{MA}_{k,n} = \frac{1}{n}\sum_{i=k-n+1}^{k} Z_i$ forms a stochastic process (starting at $k = n - 1$).

10.1.2 Markov Chains

A stochastic process is *Markov* if the next state depends (at most) on the current state and not on any earlier states, provided you know the current state. It is a *Markov chain* if it is Markov and discrete ($T \subset \mathbb{N}$).

Definition 10.1.6. *A stochastic process* $(X_t)_{t\in\mathbb{N}}$ *is a* Markov chain *if*

$$P(X_{m+1} = x_{m+1} \mid X_m = x_m, \ldots, X_0 = x_0) = P(X_{m+1} = s \mid X_m = x_m) \quad (10.1)$$

for all $m \in \mathbb{N}$ *and* $x_1, \ldots, x_{m+1} \in S$. *When confusion is unlikely, we often write just a lowercase* x_i *to denote* $X_i = x_i$, *so* (10.1) *becomes*

$$P(x_{m+1} \mid x_m, \ldots, x_0) = P(x_{m+1} \mid x_m).$$

Example 10.1.7. Any sequence $(X_t)_{t\in\mathbb{N}}$ of independent random variables is Markov, because each state is independent of all other states, thus

$$\begin{aligned} P(x_{m+1} \,\big|\, x_m, \ldots, x_0) &= P(x_{m+1}) \\ &= P(x_{m+1} \,\big|\, x_m). \end{aligned}$$

These random variables need not be identically distributed—being independent is more than enough for them to form a Markov chain.

Example 10.1.8. A random walk is Markov because $X_{m+1} = X_m + Z_{m+1}$ depends only on the previous value X_m and the random variable Z_{m+1}, which is independent of all the previous X_t for $t \leq m$. This gives

$$\begin{aligned} P(x_{m+1} \,\big|\, x_m, \ldots, x_0) &= P(Z_{m+1} = x_{m+1} - x_m \,\big|\, X_m = x_m, \ldots, X_0 = x_0) \\ &= P(Z_{m+1} = x_{m+1} - x_m \,\big|\, X_m = x_m) \\ &= P(x_{m+1} \,\big|\, x_m). \end{aligned}$$

A random walk with absorbing barriers is also Markov. Although the property of being bankrupt at time $t+1$ may depend on a much earlier situation, like having been bankrupt earlier, the amount of money the gambler has at time t completely determines the probability of being bankrupt at time $t+1$. There is no additional information about future states that is not already contained in our knowledge of the gambler's current wealth. Hence, we have

$$P(x_{t+1} \,\big|\, x_t) = P(x_{t+1} \,\big|\, x_t, x_{t-1} \ldots, x_0).$$

Figure 10.1: Image of a late 18th century cloth game board for the game Gyan Chaupar, an early version of Snakes and Ladders. The original is located in the decorative arts gallery of the National Museum, India. Acc. No. 85.312. Photograph by Nomu420, CC BY-SA 3.0 `https://creativecommons.org/licenses/by-sa/3.0`, via Wikimedia Commons.

Example 10.1.9. In the game of *Snakes and Ladders* (see Figure 10.1) players roll a die and move their pieces along the board the number of squares indicated by the die. In this way, the position of a player's piece on the board is like a random walk on the list S of squares on the board, except that if a piece goes past the last square, they win and the game is over.

However, the game also has snakes and ladders connecting various squares. If a player lands on a square with a snake head, they move their piece back to the square at the tail of the snake. If they land on a square at the bottom of a ladder, they move their piece forward to the square at the top of the ladder.

At the mth turn, the new position X_{m+1} of the player's piece is solely a function of where their piece was at the beginning of the turn (the position X_m) and the number shown on the die. Previous positions X_k for $k < m$ do influence the position X_{m+1} but they only do so by their impact on the position X_m. Thus each player's position in *Snakes and Ladders* is a Markov chain.

Moreover, the position of all the players also forms a Markov chain. If $A = \{0, \ldots, N-1\}$ is the set of all players (or, rather, the players' numbers), then the state space for all players could be $S^N = \{(s_0, \ldots, s_{N-1}) \mid s_i \in S \; \forall i \in A\}$, where s_i records the position of the ith player's piece on the board. At time $t = 0$ it is player 0's turn, and so on up to time $t = N-1$, but at time $t = N$, it returns to player 0's turn. Thus, in general, at time t it is the turn of player $t \pmod N$.

At the tth turn, state $(s_0, \ldots, s_k, \ldots, s_{N-1})$ with $t \equiv k \pmod N$ can only change to a state of the form $(s_0, \ldots, s'_k, \ldots, s_{N-1})$; that is, all the coordinates must remain unchanged except s_k (the position of player k's piece) can change to some other position on the board. The new state X_{t+1} is determined solely by k, the state X_t (where every piece is and whose turn it is) and the value on the die. Earlier states do influence X_{t+1} by influencing X_t, but once we know X_t, there is no additional information gained by knowning the earlier states.

Unexample 10.1.10. The sequence of nth moving averages in Example 10.1.5 is not Markov because $\mathrm{MA}_{k+1} = \mathrm{MA}_k + \frac{1}{n} Z_{k+1} - \frac{1}{n} Z_{k-n+1}$ is not independent of MA_{k-n} and MA_{k-n+1} (note that $Z_{k-n+1} = \mathrm{MA}_{k-n+1} - \mathrm{MA}_{k-n}$).

10.1.3 Temporally Homogenous Markov Chains

An arbitrary Markov chain could have its transition probabilities change over time; for example, we could have $P(X_2 = s \mid X_1 = r) \neq P(X_3 = s \mid X_2 = r)$. But many situations correspond to a simpler case, where the probability of moving from state r to state s is fixed for all time. We call such Markov chains *temporally homogeneous*.

Definition 10.1.11. *A Markov chain* $(X_t)_{t \in \mathbb{N}}$ *is* temporally homogeneous *if*

$$P(X_{m+k} = r \mid X_k = s) = P(X_m = r \mid X_0 = s)$$

for all $k, m \in \mathbb{N}$ *and for all* $r, s \in S$.

Example 10.1.12. A simple random walk with a coin that has probability p of heads satisfies

$$P(X_{t+1} = a \,\big|\, X_t = b) = \begin{cases} p & \text{if } a = b + 1 \\ 1 - p & \text{if } a = b - 1 \\ 0 & \text{otherwise.} \end{cases}$$

These probabilities are independent of t, so the simple random walk is temporally homogeneous.

Unexample 10.1.13. Consider a game between two players who repeatedly flip a coin. On the first turn, the winner gets \$1, on the second and third turns, the winner of each flip gets half of a dollar. On turns 4–7 the winner of each flip gets a quarter. On turns 8–15, the winner gets $\frac{1}{8}$, and at any time $t \in \{2^k, \ldots, 2^{k+1} - 1\}$, the winner of each coin flip receives 2^{-k} dollars. Let the state space be player A's wealth. The probability of moving from state s to state $s + 2^{-k}$ is zero if $t \notin \{2^k, \ldots, 2^{k+1} - 1\}$ and it is $\frac{1}{2}$ if $t \in \{2^k, \ldots, 2^{k+1} - 1\}$. Therefore, this Markov chain is not temporally homogeneous—the transition probabilities depend on the time (which turn it is).

Example 10.1.14. A simple random walk with an absorbing barrier at 0 and L satisfies

$$P(X_{t+1} = a \,\big|\, X_t = b) = \begin{cases} 1 & \text{if } a = b = 0 \text{ or } a = b = L \\ p & \text{if } a = b + 1 \text{ and } 0 < b < L \\ 1 - p & \text{if } a = b - 1 \text{ and } 0 < b < L \\ 0 & \text{otherwise.} \end{cases}$$

These values are all independent of t, so the simple random walk with absorbing barrier is temporally homogeneous.

Unexample 10.1.15. The Markov chain for the full game of *Snakes and Ladders* given in Example 10.1.9 is not temporally homogeneous because at time t a given state $(s_0, \ldots, s_k, \ldots, s_{N-1})$ with $t \equiv k \pmod{N}$ can only change to a state of the form $(s_0, \ldots, s'_k, \ldots, s_{N-1})$; that is, only the position of player k's piece may change. Thus the probability of a given transition depends on the time t. There are ways to reformulate the game as a temporally homogeneous Markov chain by enlarging the state space to include information about whose turn it is. But the Markov chain described in Example 10.1.9 for the full game is not temporally homogeneous.

The next theorem shows that in a temporally homogeneous Markov chain the probability of moving from x to z in two steps is the sum over all $y \in S$ of the probabilities of moving from x to y and then from y to z. This implies that for finite-state temporally homogeneous Markov chains the transition probabilities can be calculated by matrix multiplication.

Theorem 10.1.16 (Chapman-Kolmogorov[39]). *Assume that $(X_t)_{t\in T}$ is a temporally homogeneous Markov chain with countable state space S. Let $p_{ij}(n) = P(X_n = i \mid X_0 = j)$ be the probability of moving to state $i \in S$ from state $j \in S$ in n steps. We have*

$$p_{ij}(m+n) = \sum_{k\in S} p_{ik}(n)p_{kj}(m). \tag{10.2}$$

Proof.

$$\begin{aligned}
p_{ij}(m+n) &= \sum_{k\in S} P(X_{m+n} = i, X_m = k \mid X_0 = j) \\
&= \sum_{k\in S} P(X_{m+n} = i \mid X_m = k, X_0 = j)P(X_m = k \mid X_0 = j) \\
&= \sum_{k\in S} P(X_{m+n} = i \mid X_m = k)P(X_m = k \mid X_0 = j) \\
&= \sum_{k\in S} P(X_n = i \mid X_0 = k)P(X_m = k \mid X_0 = j) \\
&= \sum_{k\in S} p_{ik}(n)p_{kj}(m). \qquad \square
\end{aligned}$$

Corollary 10.1.17. *Assume that $(X_t)_{t\in T}$ is a temporally homogeneous Markov chain with finite state space S. If $Q(n)$ is the matrix $[Q(n)]_{ij} = p_{ij}(n) = P(X_n = i \mid X_0 = j)$, then $Q(2) = Q(1)Q(1)$, and $Q(n) = Q(1)^n$.*

Proof. The proof is Exercise 10.5. $\square$

[39] Kolmogorov (pronounced Kohl-muh-GORE-uff) founded modern measure-theoretic probability in 1933.

Remark 10.1.18. From now on, we assume that all Markov chains are temporally homogeneous, unless otherwise stated. If the state space is finite, we write $Q = Q(1)$ and call this the *transition matrix* of the Markov chain. We are interested in both the long-term behavior of Q^n when $n \gg 1$ and the transient behavior of Q^n when n is not yet large.

Remark 10.1.19. The jth column of Q consists of the probabilities of transitioning from j to each of the other states, therefore $Q \succeq 0$ and each column must sum to 1 (such a matrix is called *column stochastic*). Exercise 10.4 shows that the spectral radius of any column-stochastic matrix is 1.

Nota Bene 10.1.20. Beware that some authors use the convention for the transition matrix of $Q_{ij} = P(X_1 = j \mid X_0 = i)$, which makes their transition matrix equal to our Q^{T}. This has the disadvantage of requiring the distributions for X_t to be represented as row vectors with the transition matrix acting on the right, which is logically equivalent to our convention, but awkward for anyone that is used to writing vectors as columns and using matrices that act on the left.[a]

[a]Using row vectors is sort of like insisting on using the British imperial measurement system (yards, pints, pounds, and slugs) when everyone around you is using the metric system (meters, liters, Newtons, and grams); see also `https://www.youtube.com/watch?v=JYqfVE-fykk`.

In a finite-state Markov chain with state space $S = \{1, \ldots, n\}$, the probability distribution for X_0 can be written as a vector $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_n)$, where $\pi_k = P(X_0 = k)$ for each state $k \in S$ and $\sum_{k=1}^{n} \pi_k = 1$.

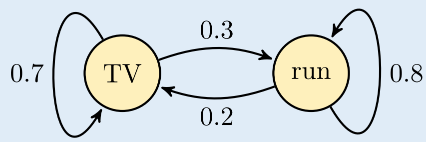
Proposition 10.1.21. *In a finite-state Markov chain with state space $S = \{1, \ldots, n\}$ and probability distribution $\boldsymbol{\pi}$ for X_0, the marginal distribution of X_1 (that is, the distribution of X_1 without regard for the other X_t), is $Q\boldsymbol{\pi}$, meaning that $P(X_1 = k) = (Q\boldsymbol{\pi})_k$.*

Proof. The proof is Exercise 10.6. ∎

10.1.4 Transition Diagrams

If the state space of a Markov chain is finite, then we can depict the Markov chain with a weighted directed graph, where the nodes are the states, and an edge is drawn from s to s' if $P(X_{m+1} = s' \mid X_m = s) > 0$. The weight on an edge (s, s') is $p_{s's}$. This graph is sometimes called the *transition diagram* for the Markov chain. The probability-weighted adjacency matrix for the transition diagram is the transpose Q^{T} of the transition matrix. This means that the probability of moving from state s to state s' in t steps is $(Q^t)_{s's}$.

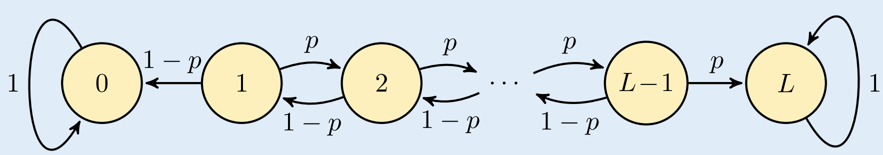
Example 10.1.22. I try to stay fit by going for a run every evening, but I don't always have the discipline to do this. Sometimes I watch TV instead. If I do run, I feel good afterwards and that makes me more inclined to run again the next day. My probability of running today if I ran yesterday is 80% (and the probability of watching TV today is 20%). Similarly if I watch TV, I feel sluggish and less inclined to run the next day. My probability of running today, if I watched TV yesterday is only 30% (and my probability of watching TV again is 70%). Here is the transition diagram for a Markov chain modeling my evening activities.



If TV is the first state and run is the second, then the transition matrix is

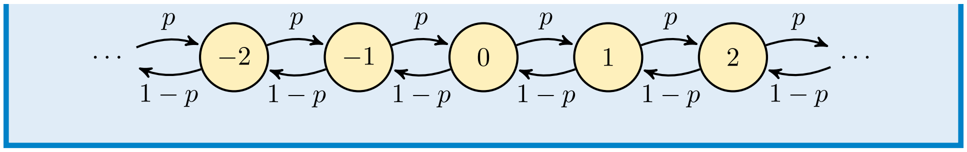
$$Q = \begin{bmatrix} 0.7 & 0.2 \\ 0.3 & 0.8 \end{bmatrix}.$$

Example 10.1.23. A simple random walk with absorbing barriers at 0 and L has the following transition diagram



When the state space of the Markov chain is infinite, but discrete, we construct an infinite directed graph as the transition diagram, analogous to the finite case.

Example 10.1.24. A simple random walk (with no barriers) has the following infinite transition diagram.



10.1.5 *Gaps in Conditioning

Throughout this section, let $(X_t)_{t\in\mathbb{N}}$ be a Markov chain on $(\Omega, \mathscr{F}, P)$ with state space S. In a Markov chain a relation similar to (10.1) holds when some of the intermediate terms are left out of the conditioning. First consider the case where a string of middle terms is left out of the conditioning. In the following proposition, the terms $x_{m+1}, x_{m+2}, \dots, x_{m+k-2}$ are all missing.

Proposition 10.1.25. *For any $k, m \in \mathbb{N}$ with $k \geq 1$, and for any $x_0, \dots, x_m, x_{m+k} \in S$, we have*

$$P(x_{m+k} \,|\, x_{m+k-1}, x_m, \dots, x_0) = P(x_{m+k} \,|\, x_{m+k-1}). \tag{10.3}$$

Proof. Let $C = \{X_m = x_m, \dots, X_0 = x_0\}$. In the following expressions, the sum $\sum_{\mathbf{s}}$ is taken over all choices of $\mathbf{s} = (s_{m+1}, s_{m+2}, \dots, s_{m+k-2}) \in S^{k-2}$. We have

$$\begin{aligned}
&P(x_{m+k} \,|\, x_{m+k-1}, C) \\
&\quad = P(x_{m+k} \,|\, x_{m+k-1}, X_{m+k-2} \in S, \dots, X_{m+1} \in S, C) \\
&\quad = \frac{P(x_{m+k}, x_{m+k-1}, X_{m+k-2} \in S, \dots, X_{m+1} \in S, C)}{P(x_{m+k-1}, X_{m+k-2} \in S, \dots, X_{m+1} \in S, C)} \\
&\quad = \frac{\sum_{\mathbf{s}} P(x_{m+k}, x_{m+k-1}, s_{m+k-2}, \dots, s_{m+1}, C)}{P(x_{m+k-1}, X_{m+k-2} \in S, \dots, X_{m+1} \in S, C)} \\
&\quad = \frac{\sum_{\mathbf{s}} P(x_{m+k} \,|\, x_{m+k-1}, s_{m+k-2}, \dots, s_{m+1}, C) P(x_{m+k-1}, s_{m+k-2}, \dots, s_{m+1}, C)}{P(x_{m+k-1}, X_{m+k-2} \in S, \dots, X_{m+1} \in S, C)} \\
&\quad = \frac{P(x_{m+k} \,|\, x_{m+k-1}) \sum_{\mathbf{s}} P(x_{m+k-1}, s_{m+k-2}, \dots, s_{m+1}, C)}{P(x_{m+k-1}, X_{m+k-2} \in S, \dots, X_{m+1} \in S, C)} \\
&\quad = \frac{P(x_{m+k} \,|\, x_{m+k-1}) P(x_{m+k-1}, X_{m+k-2} \in S, \dots, X_{m+1} \in S, C)}{P(x_{m+k-1}, X_{m+k-2} \in S, \dots, X_{m+1} \in S, C)} \\
&\quad = P(x_{m+k} \,|\, x_{m+k-1}). \qquad \square
\end{aligned}$$

The second case is when the gap is at the top of the range. In the next proposition all the values $x_{m+1}, \dots, x_{m+k-1}$ are missing.

Proposition 10.1.26. *For any $m, k \in \mathbb{N}$ with $k \geq 1$, and any $x_0, \dots, x_m, x_{m+k} \in S$, we have*

$$P(x_{m+k} \mid x_m, \dots, x_0) = P(x_{m+k} \mid x_m).$$

Proof. We proceed by induction. The $k = 1$ case holds by (10.1.6). Let $C = \{X_m = x_m, \dots, X_0 = x_0\}$. The inductive hypothesis gives

$$P(X_{m+k-1} = s \,|\, C) = P(X_{m+k-1} = s \,|\, x_m),$$

for all $s \in S$. Equation (10.3) gives

$$P(X_{m+k} = x_{m+k} \mid X_{m+k-1} = s, C) = P(X_{m+k} = x_{m+k} \mid X_{m+k-1} = s).$$

Thus,

$$\begin{aligned}
P(X_{m+k} = x_{m+k} \mid C) &= \sum_{s \in S} P(X_{m+k} = x_{m+k}, X_{m+k-1} = s \mid C) \\
&= \sum_{s \in S} P(X_{m+k} = x_{m+k} \mid X_{m+k-1} = s) P(X_{m+k-1} = s \mid X_m = x_m) \\
&= \sum_{s \in S} P(X_{m+k} = x_{m+k} \mid X_{m+k-1} = s, X_m = x_m) P(X_{m+k-1} = s \mid X_m = x_m) \\
&= \sum_{s \in S} P(X_{m+k} = x_{m+k}, X_{m+k-1} = s \mid X_m = x_m) \\
&= P(x_{m+k} \mid x_m). \quad \square
\end{aligned}$$

And more generally, we have the following proposition.

Proposition 10.1.27. *For any nonnegative integers $n_1 < n_2 < \cdots < n_k \leq n$, and any $x_{n_1}, \ldots, x_{n_k}, x_n \in S$, we have*

$$P(X_n = x_n \mid X_{n_k} = x_{n_k}, \ldots, X_{n_1} = x_{n_1}) = P(X_n = x_n \mid X_{n_k} = x_{n_k}).$$

Proof. The proof is Exercise 10.7. $\square$

10.2 Irreducible Markov Chains and Stationary Distributions

In this section we define several natural properties of a Markov chain and its states, and we show that for Markov chains with a finite state space, these properties correspond to important properties of the transition matrix Q of the Markov chain. These results will be especially important when we study MCMC.

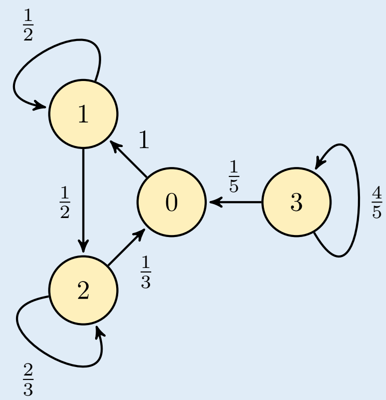
Throughout this section we assume that $(X_t)_{t \in \mathbb{N}}$ is a (temporally homogeneous) Markov chain on a probability space $(\Omega, \mathscr{F}, P)$ with discrete state space S.

10.2.1 Classification of States

The states of a Markov chain can be separated into two types—those that are *recurrent*, meaning that they keep coming up, over and over, and those that are not recurrent (called *transient*). These definitions are made mathematically precise below.

Definition 10.2.1. *A state $s' \in S$ is* accessible *from state $s \in S$ if there exists some $n \in \mathbb{N}$ such that $p_{s's}(n) > 0$. A state s is* recurrent *if for every state s' that is accessible from s, the state s is accessible from s'; that is, starting at s, at every stage thereafter there is a nonzero probability of returning to s. A state is* transient *if it is not recurrent.*

Example 10.2.2. For a Markov chain with the following transition diagram, the state 3 is transient because 0 is accessible from 3 (there is a nonzero probability of moving from 3 to 0), but 3 is not accessible from 0 (no probability of ever returning to 3 from 0). The states 0, 1, and 2 are all recurrent.



Example 10.2.3. In a simple random walk with absorbing barriers (see Example 10.1.23), every state in $S = \{0, \ldots, L\}$ is accessible from the states $\{1, \ldots, L-1\}$. But the only state accessible from 0 is 0 and the only state accessible from L is L. The states 0 and L are recurrent, but the states $\{1, \ldots, L-1\}$ are transient, because they are not accessible from the barrier states 0 and L, which are, themselves both accessible from each state in $\{1, \ldots, L-1\}$.

Proposition 10.2.4. *For any given Markov chain, the relation* is accessible from *is an equivalence relation on the set of all recurrent states.*

Proof. The proof is Exercise 10.8. □

Proposition 10.2.5. *For any given state i in a finite-state Markov chain, there must be at least one recurrent state j that is accessible from i.*

Proof. Assume, by way of contradiction, that there exists a finite-state Markov chain with a state i having no recurrent states accessible from i. The state i cannot be recurrent, because it is accessible from itself. Because i is transient, there must be a state $i_1 \neq i$ such that i_1 is accessible from i, but i is not accessible from i_1. By hypothesis, i_1 cannot be recurrent. Repeating the argument for i_1 shows that there is an $i_2 \notin \{i, i_1\}$ such that i_2 is transient and such that neither i nor i_1 is accessible from i_2. Continuing in this manner gives an infinite sequence of distinct states $i, i_1, i_2, \ldots$, but this contradicts the fact that the state space is finite. □

Proposition 10.2.6. *In a finite-state Markov chain, starting at a recurrent state i, the probability of eventually returning to i is 1. But for any transient state k, starting at k gives a nonzero probability of never returning to k.*

Proof. Starting at a recurrent state i, the only possible future states are those in the recurrence class of i. Without loss of generality, we may assume that there is only one recurrence class. It suffices to show that for any state $j \neq i$ in the recurrence class of i, starting at j, the probability of eventually returning to i is 1. Construct a new Markov chain from the recurrence class by setting $p_{ii}^{\text{new}} = 1$ and $p_{ki}^{\text{new}} = 0$ for all $k \neq i$, and leaving all other transition probabilities unchanged. Starting at $j \neq i$, the probability of eventually reaching i in the new Markov chain is the same as the probability of eventually reaching i in the original Markov chain. Moreover, in the new Markov chain, all states are transient except i, which is recurrent. By Proposition 10.2.5, starting at any $j \neq i$ one must eventually arrive at a recurrent state, but this must be i, since i is the only recurrent state. Therefore the probability of eventually reaching i is 1.

The proof that there is a nonzero probability of never returning to a transient state k is Exercise 10.9. □

10.2.2 Irreducible Markov Chains

Definition 10.2.7. *A Markov chain is called* irreducible *if for every $s, s' \in S$ there exists $k \in \mathbb{Z}^+$ such that $P(X_k = s \mid X_0 = s') > 0$. In particular, if the state space is finite, then the Markov chain is irreducible if and only if the transition matrix Q is irreducible (see Volume 1, Definition 12.8.9).*

Example 10.2.8. The Markov chain of Example 10.1.22 is irreducible because the transition matrix Q is positive, hence $P(X_1 = s \mid X_0 = s') > 0$ for all $s, s' \in S$.

Unexample 10.2.9. The simple random walk with absorbing barriers (see Example 10.1.23) is not irreducible, because $P(X_k = 1 \,|\, X_0 = 0) = 0$ for all $k \in \mathbb{Z}^+$.

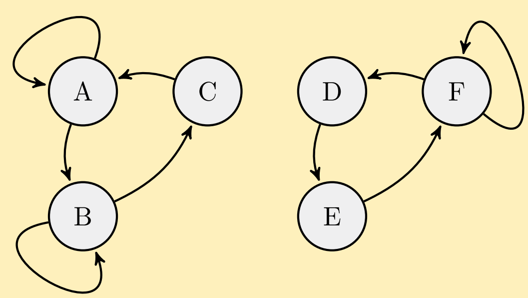
Example 10.2.10. The simple random walk (see Example 10.1.24) has an infinite state space, but it is still irreducible. To see this observe that if $s > s'$, then letting $k = s - s'$ gives $P(X_k = s \,|\, X_0 = s') \geq p^k > 0$, since one way to get from s' to s is just to move to the right k times. Similarly, if $s < s'$, then letting $k = s' - s$ gives $P(X_k = s \,|\, X_0 = s') \geq (1-p)^k > 0$. Finally, if $s = s'$, then $P(X_2 = s \,|\, X_0 = s) = 2p(1-p) > 0$ (move out and back in either direction).

Proposition 10.2.11. *A Markov chain is irreducible precisely when it has only one recurrence class and every state is recurrent.*

Proof. The proof is Exercise 10.10. ∎

Unexample 10.2.12. State 3 in the Markov chain of Example 10.2.2 is transient, hence that Markov chain cannot be irreducible, by Proposition 10.2.11.

Unexample 10.2.13. Consider a Markov chain with the following transition diagram (for each node all outgoing edges have the same probability).



Athough every state in this Markov chain is recurrent, the chain is not irreducible because it has two recurrence classes, $\{A, B, C\}$ and $\{D, E, F\}$.

Taking more and more steps in a Markov chain, the probability of ending in a transient state goes to zero, and the only states likely to occur are the recurrent states. If we discard all the transient states and consider the resulting Markov chain, it breaks into recurrence classes. Moreover, no matter which recurrence class we start in, we always remain in that class, so all other recurrence classes are irrelevant at that point—we need only consider the class in which we started. Restricting to one recurrence class and discarding all the states not in that class gives a new Markov chain that is irreducible because every state in it is recurrent and they all belong to the same recurrence class.

10.2.3 Stationary Distribution

Definition 10.2.14. *A distribution* $\boldsymbol{\pi}$ *for* X_t *is called* stationary *if the resulting (marginal) distribution for* X_{t+1} *is also* $\boldsymbol{\pi}$*.*

In a Markov chain with a countable number of states, the law of total probability gives

$$P(X_{t+1} = s') = \sum_{s \in S} P(X_{t+1} = s' \,\big|\, X_t = s) P(X_t = s) = \sum_{s \in S} P(X_{t+1} = s' \,\big|\, X_t = s) \pi_s.$$

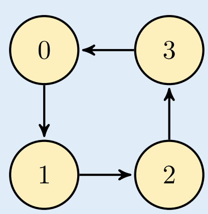
Therefore, $\boldsymbol{\pi}$ is stationary if $\sum_{s \in S} P(X_{t+1} = s' \,\big|\, X_t = s)\pi_s = \pi_{s'}$.

In the special case that the Markov chain has a finite state space and transition matrix Q, this implies that $\boldsymbol{\pi}$ is stationary if and only if

$$Q\boldsymbol{\pi} = \boldsymbol{\pi};$$

that is, $\boldsymbol{\pi}$ is stationary if and only if $\boldsymbol{\pi}$ is an eigenvector of Q with eigenvalue 1.

Example 10.2.15. Consider a Markov chain with the following transition diagram, where every arrow has probability 1.



The distribution $\boldsymbol{\pi} = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ is stationary for this Markov chain because

$$Q\boldsymbol{\pi} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{bmatrix} = \begin{bmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{bmatrix} = \boldsymbol{\pi}.$$

Example 10.2.16. The Markov chain in Example 10.2.2 has transition matrix

$$Q = \begin{bmatrix} 0 & 0 & \frac{1}{3} & \frac{1}{5} \\ 1 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & \frac{2}{3} & 0 \\ 0 & 0 & 0 & \frac{4}{5} \end{bmatrix}.$$

The distribution $\boldsymbol{\pi} = (\frac{1}{6}, \frac{1}{3}, \frac{1}{2}, 0)$ is stationary because $Q\boldsymbol{\pi} = \boldsymbol{\pi}$.

Example 10.2.17. The distributions $(1, 0, \dots, 0)$ and $(0, \dots, 0, 1)$ are both stationary distributions of the simple random walk with absorbing boundaries at 0 and L. Thus, stationary distributions need not be unique.

Proposition 10.2.18. *If a finite-state Markov chain has a symmetric transition matrix, then the uniform distribution is stationary.*

Proof. Any finite-state Markov chain is column stochastic, meaning that $\mathbb{1}^\mathsf{T} Q = \mathbb{1}^\mathsf{T}$. If the total number of states is n and Q is symmetric, then we have

$$Q\left(\frac{1}{n}\mathbb{1}\right) = \frac{1}{n}\left(\mathbb{1}^\mathsf{T} Q\right)^\mathsf{T} = \frac{1}{n}(\mathbb{1}^\mathsf{T})^\mathsf{T} = \frac{1}{n}\mathbb{1},$$

which guarantees that the uniform distribution is stationary for Q. □

10.2.4 *Mean Recurrence Time

If $\boldsymbol{\pi}$ is the stationary distribution of an irreducible Markov chain, then the percentage of the time that the chain spends in state s is π_s. This suggests that whenever the chain starts in state s, the time it takes to return to state s should be $\frac{1}{\pi_s}$ on average. The expected time to return is called the *mean recurrence time* of state s. The following theorem guarantees that this heuristic argument gives the correct value of the mean recurrence time.

Theorem 10.2.19. *Let $\boldsymbol{\pi}$ be the stationary distribution of an irreducible Markov chain. If T_s is the random variable $T_s = \min\{t \geq 1 : X_t = s\}$, then $\mathbb{E}[T_s \mid X_0 = s] = \frac{1}{\pi_s}$.*

Proof. First note for any integer-valued random variable $Y \geq 1$ we always have

$$\mathbb{E}[Y] = \sum_{n \geq 1} P(Y \geq n). \tag{10.4}$$

This follows from an argument similar to that used to prove Exercise 8.2 (write the right side as a double sum and change the order of summation).

Now to prove the theorem: for any $s \in S$ we have

$$\begin{aligned}\mathbb{E}[T_s \mid X_0 = s]\,\pi_s &= \mathbb{E}[T_s \mid X_0 = s] P(X_0 = s) \\ &= \sum_{n\geq 1} P(T_s \geq n \mid X_0 = s) P(X_0 = s) \\ &= \sum_{n \geq 1} P(T_s \geq n, X_0 = s). \end{aligned} \tag{10.5}$$

In the case that $n = 1$, we have $P(T_s \geq 1, X_0 = s) = P(X_0 = s) = \pi_s$. In the case that $n \geq 2$ we have

$$\begin{aligned}P(T_s \geq n, X_0 = s) &= P(X_0 = s, X_j \neq s \;\forall 1 \leq j \leq n-1) \\ &= P(X_j \neq s \;\forall 1 \leq j \leq n-1) - P(X_j \neq s \;\forall 0 \leq j \leq n-1) \\ &= P(X_j \neq s \;\forall 0 \leq j \leq n-2) - P(X_j \neq s \;\forall 0 \leq j \leq n-1)\end{aligned}$$

The last equality follows from the fact that $\boldsymbol{\pi}$ is stationary. Setting $a_k = P(X_j \neq s \;\forall 0 \leq j \leq k)$ transforms the previous equation into

$$P(T_s \geq n, X_0 = s) = a_{n-2} - a_{n-1}.$$

Combining this with (10.5) gives a telescoping sum

$$\mathbb{E}[T_s \mid X_0 = s]\,\pi_s = \pi_s + \sum_{n\geq 2} (a_{n-2} - a_{n-1}) = \pi_s + a_0 - \lim_{n\to\infty} a_n. \tag{10.6}$$

Observe that

$$a_0 = P(X_0 \neq s) = 1 - \pi_s. \tag{10.7}$$

Moreover, because s is recurrent Proposition 10.2.6 implies that

$$\lim_{n\to\infty} a_n = P(X_j \neq s \;\forall j) = 0. \tag{10.8}$$

Combining 10.6, 10.7, and 10.8 gives

$$\mathbb{E}[T_s \mid X_0 = s]\,\pi_s = \pi_s + a_0 - \lim_{n\to\infty} a_n = 1.$$

Therefore $\mathbb{E}[T_s \mid X_0 = s] = \frac{1}{\pi_s}$, as desired. □

10.3 Existence and Uniqueness of Stationary Distributions

A finite-state irreducible Markov chain always has a unique stationary distribution.

Proposition 10.3.1. *Every irreducible, finite-state Markov chain has a unique stationary distribution.*

Proof. If a finite-state Markov chain is irreducible, then its transition matrix Q is irreducible. By the Perron-Frobenius theorem (Volume 1, Theorem 12.8.11) any irreducible Q has a positive eigenvector $\boldsymbol{\pi}$ corresponding to the eigenvalue 1. Rescaling $\boldsymbol{\pi}$ so that $\sum_{i=1}^{n} \pi_i = 1$ gives a stationary distribution for the Markov chain. Perron-Frobenius guarantees that the eigenvalue is simple, so its eigenspace has dimension one. This implies that every corresponding eigenvector is a multiple of $\boldsymbol{\pi}$ and thus every stationary distribution must equal $\boldsymbol{\pi}$. ∎

Unexample 10.3.2. Consider the simple random walk with no boundaries (see Example 10.1.24) in the special case where $p = \frac{1}{2} = 1 - p$. If there were a stationary distribution $\boldsymbol{\pi}$ for this Markov chain, then for any $s \in \mathbb{Z}$ we would have

$$\pi_s = \frac{1}{2}\pi_{s-1} + \frac{1}{2}\pi_{s+1} \qquad \text{and} \qquad \pi_{s+1} = 2\pi_s - \pi_{s-1}.$$

This gives

$$\pi_2 = 2\pi_1 - \pi_0,\ \pi_3 = 3\pi_1 - 2\pi_0,\ \ldots,$$

which gives

$$\pi_s = s\pi_1 - (s-1)\pi_0 \qquad \forall s \in \mathbb{Z}. \tag{10.9}$$

But since $0 \leq \pi_s \leq 1$, this gives $0 \leq s\pi_1 - (s-1)\pi_0$ and

$$\left(1 - \frac{1}{s}\right)\pi_0 \leq \pi_1 \leq \frac{1}{s} - \left(1 - \frac{1}{s}\right)\pi_0 \qquad \forall s \in \mathbb{Z}.$$

Taking the limit as $s \to \infty$ gives $\pi_0 = \pi_1$. Combining this with (10.9) shows that $\pi_s = \pi_0$ for all $s \in \mathbb{Z}$. But this contradicts the requirement that $\sum_{s \in \mathbb{Z}} \pi_s = 1$.

Therefore this simple random walk with no boundaries has no stationary distribution, despite the fact that it is irreducible. This does not contradict Proposition 10.3.1 because it has an infinite state space, and the proposition only holds for finite-state Markov chains.

For a Markov chain with a small state space and transition matrix Q, the stationary distribution can be found using standard methods for finding the eigenvector of Q corresponding to the eigenvalue 1. But if the state space is very large (for example, one state for each website on the internet), then standard matrix methods are too expensive. Fortunately, there are other ways to compute the stationary distribution.

The power method (Volume 1, Theorem 12.7.8) gives an algorithm for finding the stationary distribution of a finite-state Markov chain in many cases, as described in the following theorem.

Theorem 10.3.3. *Consider a finite-state Markov chain with transition matrix Q such that the only eigenvalue of Q on the unit circle in $\mathbb{C}$ is the eigenvalue 1. For any initial distribution $\mathbf{v}$ (a nonnegative vector $\mathbf{v}$ with $\|\mathbf{v}\|_1 = 1$) such that $\mathrm{Pr}_1 \mathbf{v} \neq \mathbf{0}$, where Pr_1 is the eigenprojection onto the eigenspace corresponding to eigenvalue 1, if $\boldsymbol{\pi}$ is the stationary distribution, then we have*

$$\|Q^k \mathbf{v} - \boldsymbol{\pi}\| \to 0$$

as $k \to \infty$.

Proof. This follows from the power method (Volume 1, Theorem 12.7.8). ∎

Remark 10.3.4. Although Perron-Frobenius guarantees that 1 is a simple eigenvalue, it does not prevent the existence of another eigenvalue on the unit circle in $\mathbb{C}$. Below we describe an additional property (aperiodicity) of some Markov chains that guarantees this cannot happen.

The theorem shows that one way to find the stationary distribution of a finite-state irreducible Markov chain with no other eigenvalues on the unit circle is to simply choose a random vector $\mathbf{v}$ and compute $Q^k\mathbf{v}$ for $k \to \infty$, and the result will converge to the stationary distribution $\boldsymbol{\pi}$. The theorem fails in the case that $\mathbf{v}$ happens to lie in the kernel of the projection Pr_1, but the probability that a randomly chosen vector will lie in that kernel is 0, so it is not usually a problem. In the very rare case where the sequence does not seem to be converging, restarting with a different $\mathbf{v}$ usually solves the problem.

If the number of states is very large, then computing $Q^k\mathbf{v}$ may still seem difficult, but if Q is sparse with only m nonzero entries and $\mathbf{v}$ is dense with $n = |S|$ entries, then the complexity of the matrix-vector multiplication is only $O(m + n)$. Even if the matrix Q is not sparse, when it has special structure (for example, the Google PageRank matrix) then $Q^k\mathbf{v}$ can still be calculated efficiently.

10.3.1 Aperiodicity

The condition in Theorem 10.3.3 that no other eigenvalues of the transition matrix may lie on the unit circle is important. Markov chains that have the property of being *aperiodic* are guaranteed to have no other eigenvalues on the unit circle.

Definition 10.3.5. *The* period *of a state s in a Markov chain is the greatest common divisor of the lengths of all closed walks in the chain that start and end at s. A state is* periodic *if its period is greater than* 1 *and* aperiodic *if its period is* 1*. A Markov chain is* aperiodic *if all its states are aperiodic.*

Unexample 10.3.6. Every state in the Markov chain of Example 10.2.15 has period 4. Therefore, this chain is not aperiodic. The transition matrix has eigenvalues 1, i, -1, and $-i$, all of which lie on the unit circle. Moreover, the transition matrix just rotates the states, so for any $\mathbf{v}$ and any $k \equiv 0 \pmod 4$ we have $Q^k\mathbf{v} = \mathbf{v}$. Thus the power method does not converge for this Markov chain.

Example 10.3.7. The Markov chain in Unexample 10.2.13 is aperiodic. In particular, states A, B and F all begin and end a closed walk of length one, so their periods are 1. State C begins and ends a closed walk of length three (C,A,B,C) and length four (C,A,A,B,C) and $\gcd(3,4) = 1$ so the period of state C is 1. Similarly, states D and E both begin and end closed walks of length three and four, so their period is also $\gcd(3,4) = 1$. Since all states are aperiodic, the chain is also aperiodic.

Theorem 10.3.8. *A finite-state, irreducible Markov chain is aperiodic if and only if its transition matrix Q is primitive, that is, if there exists some $k \in \mathbb{Z}^+$ such that $Q^k \succ 0$ (see Volume 1 Definition 12.8.9).*

Proof. Assume the Markov chain is aperiodic. Each state $s \in S$ is aperiodic; hence there exist closed walks starting and ending at s of lengths $\ell_1, \ldots, \ell_m$ with $\gcd(\ell_1, \ldots, \ell_m) = 1$. Let L_s be the set of all possible lengths of closed walks starting and ending at s. By the lemma below (Lemma 10.3.9), there exists a number $N_s > 0$ so that every number $n \geq N$ lies in L_s. Since Q is irreducible, for any other state $s' \in S$, there exists $k_{ss'}$ such that $(Q^{k_{ss'}})_{ss'} > 0$; thus, there exists a walk from s' to s of length $k_{ss'}$. Combining this walk with a closed walk from s shows that for any $k > N_s + k_{ss'}$ there is a walk from s' to s of length k, and hence $(Q^k)_{ss'} > 0$. Taking $K \geq \max_{s\in S}(N_s + \max_{s'\in S} k_{ss'})$ shows that $Q^k \succ 0$ for all $k \geq K$, and hence Q is primitive.

The proof of the converse (If Q is primitive, then the chain is aperiodic) is Exercise 10.15. □

To finish the proof, we need the following lemma.

Lemma 10.3.9. *For any subset $\{\ell_1, \ldots, \ell_m\} \subset \mathbb{Z}^+$ let $L = \{\sum_{i=1}^m y_i\ell_i \neq 0 \mid y_i \in \mathbb{N}\,\forall i\}$ be the set of all nonzero linear combinations of the ℓ_i obtained with only nonnegative integer coefficients. If $\gcd(\ell_1, \ldots, \ell_m) = 1$ there exists a $k > 0$ such that any $n > k$ lies in L.*

Proof. Observe first that any nonzero sum of the form $\sum_{i=1}^m y_i a_i$ is in L if the y_i are all nonnegative and the a_i are all in L.

Since the ℓ_i are relatively prime, there exist integers $z_1, \ldots, z_m$ such that $\sum_{i=1}^m z_i\ell_i = 1$ (see Volume 2, Theorem 1.8.9). Some of the z_i are negative, but moving all the negative terms to the right gives

$$\sum_{i:z_i\geq 0} z_i\ell_i = 1 + \sum_{i:z_i<0} (-z_i)\ell_i.$$

Let $w = \sum_{i:z_i<0}(-z_i)\ell_i$, and note that $w \in L$, as is $w + 1 = \sum_{i:z_i\geq 0} z_i\ell_i$. We claim that if $k = w^2 - 1$, then any $n \geq k$ is in L. To see this, use the division algorithm (Volume 2, Theorem 1.8.6) to write $n = qw + r$ with $0 \leq r < w$. Since $n \geq w^2 - 1 = w(w-1) + (w-1)$ we have $q \geq w - 1 \geq r$ and

$$n = qw + r = (q-r)w + rw + r = (q-r)w + r(w+1).$$

Since both w and $w+1$ lie in L, this shows that n also lies in L. □

Corollary 10.3.10. *A finite-state, aperiodic, irreducible Markov chain has no eigenvalues on the unit circle except the eigenvalue* 1*, and its stationary distribution can be computed by the power method.*

Proof. The proof is Exercise 10.16 □

10.3.2 Reversibility

Sometimes we are given a distribution $\boldsymbol{\pi}$ that we would like to show is stationary, but it is difficult to check the relation $Q\boldsymbol{\pi} = \boldsymbol{\pi}$. This happens, for example, when the matrix Q is enormously big. The following property is stronger than stationarity, but it is often much easier to check.

Definition 10.3.11. *In a Markov chain with a countable state space S, a distribution $\boldsymbol{\pi}$ on the states is called* reversible *if it satisfies the* detailed balance equations*, namely, if for every pair of states $r, s \in S$ we have*

$$\pi_s P(X_{t+1} = r \,|\, X_t = s) = \pi_r P(X_{t+1} = s \,|\, X_t = r). \tag{10.10}$$

Remark 10.3.12. If the Markov chain has a finite state space S and transition matrix Q, then the detailed balance equations can be written

$$Q_{rs}\pi_s = Q_{sr}\pi_r \qquad \forall r, s \in S.$$

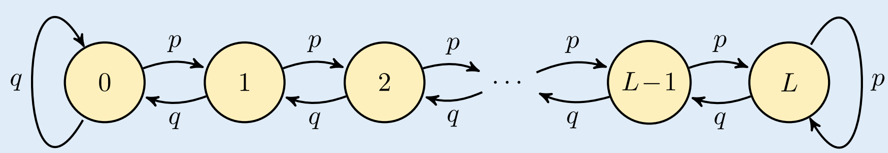
Proposition 10.3.13. *In a Markov chain with a countable state space S, a reversible distribution is stationary.*

Proof. Summing the detailed balance equations (10.10) over all states $s \in S$, and using Chapman-Kolmogorov gives

$$\begin{aligned} P(X_{t+1} = r) &= \sum_s \pi_s P(X_{t+1} = r \,|\, X_t = s) \\ &= \sum_s \pi_r P(X_{t+1} = s \,|\, X_t = r) \\ &= \pi_r \sum_s P(X_{t+1} = s \,|\, X_t = r) = \pi_r. \end{aligned}$$

This holds for all $r \in S$, which is exactly the condition for stationarity. ◻

Example 10.3.14. Consider a Markov chain with the following transition diagram, where $p + q = 1$:



For each $i \in \{0, \dots, L\}$ let $\varpi_i = (\frac{p}{q})^i$. This is not a distribution, because $\sum_i \varpi_i \neq 1$. But setting $Z = \sum_i \varpi_i$, and rescaling all the ϖ_i to $\pi_i = \frac{\varpi_i}{Z}$ for all $i \in \{1, \dots, L\}$ makes $\boldsymbol{\pi} = (\pi_1, \dots, \pi_L)$ a distribution. Moreover, $\boldsymbol{\pi}$ satisfies the detailed balance equations because

$$\pi_i Q_{i+1,i} = \frac{p}{Z}\left(\frac{p}{q}\right)^i = \frac{q}{Z}\left(\frac{p}{q}\right)^{i+1} = \pi_{i+1} Q_{i,i+1}$$

and

$$\pi_i Q_{ji} = 0 = \pi_j Q_{ij} \qquad \forall j \notin \{i-1, i+1\},$$

Example 10.3.15. Given a finite undirected graph, construct a Markov chain by setting the transition probability from vertex v to a neighboring vertex u to be $\frac{1}{d_v}$, where d_v is the number of edges connecting to v (if an edge is a loop connecting both ends to the same vertex, then count both ends of the loop). let N be the total number of edges in the graph. The vector $\boldsymbol{\pi}$ which has $\pi_v = \frac{d_v}{2N}$ for each vertex v is reversible because

$$\pi_v P(X_{t+1} = u \,|\, X_t = v) = \frac{d_v}{2N}\frac{1}{d_v} = \frac{1}{2N} = \frac{d_u}{2N}\frac{1}{d_u} = \pi_u P(X_{t+1} = v \,|\, X_t = u).$$

Therefore $\boldsymbol{\pi}$ is a stationary distribution.

Example 10.3.16. We can generalize Example 10.3.15 to the situation where the edges are weighted. Assume the edge between vertex j and vertex i has weight w_{ij}, with $w_{ij} = w_{ji}$ (symmetric). Let the transition probability from vertex j to vertex i be given by

$$Q_{ij} = \frac{w_{ij}}{\sum_k w_{kj}}.$$

This Markov chain is called a random walk on the weighted graph. Let $Z = \sum_{i,j} w_{ij}$ be the sum of all the weights, and for each i let $\pi_i = \frac{\sum_k w_{ki}}{Z}$. The distribution $\boldsymbol{\pi}$ on the vertices defined by the π_i satisfies the detailed balance equations

$$\pi_j Q_{ij} = \frac{\sum_k w_{kj}}{Z}\frac{w_{ij}}{\sum_k w_{kj}} = \frac{1}{Z}w_{ij} = \frac{\sum_k w_{ki}}{Z}\frac{w_{ji}}{\sum_k w_{ki}} = \pi_i Q_{ji}.$$

Thus, $\boldsymbol{\pi}$ is reversible, hence stationary.

10.4 *Simple Random Walks and Gambler's Ruin

10.4.1 Simple Random Walks

Definition 10.4.1. *Consider the sequence $(X_i)_{i=1}^{\infty}$ of independent Bernoulli random variables with parameter p, where the codomain of each X_i is $\{-1, 1\}$; that is, $P(X_i = 1) = p$ and $P(X_i = -1) = q = 1 - p$. Define the sequence of partial sums $S_n = S_0 + \sum_{i=1}^{n} X_i$, where S_0 is a constant or a random variable independent of each X_i. The sequence $(S_n)_{i=0}^{\infty}$ is called a* simple random walk.

Proposition 10.4.2. *If X, Y are independent random variables, then*

$$P(X + Y = b \mid Y = a) = P(X = b - a).$$

Proof. Note that $\{X+Y=b\} \cap \{Y=a\} = \{X=b-a\} \cap \{Y=a\}$. Thus,

$$\begin{aligned} P(X+Y=b \mid Y=a) &= \frac{P(X+Y=b, Y=a)}{P(Y=a)} = \frac{P(X=b-a, Y=a)}{P(Y=a)} \\ &= \frac{P(X=b-a)P(Y=a)}{P(Y=a)} = P(X=b-a). \quad \square \end{aligned}$$

Proposition 10.4.3. *S_n is* spatially homogeneous*; that is,*

$$P(S_n = b \mid S_0 = a) = P(S_n = b+c \mid S_0 = a+c).$$

Proof. Both sides can be reduced to $P(\sum_{i=1}^{n} X_i = b-a)$. $\square$

Proposition 10.4.4. *S_n is* temporally homogeneous*; that is,*

$$P(S_n = b \mid S_0 = a) = P(S_{m+n} = b \mid S_m = a).$$

Proof.

$$\begin{aligned} P(S_n = b \mid S_0 = a) &= P\left(\textstyle\sum_{i=1}^{n} X_i = b-a\right) = P\left(\textstyle\sum_{j=m+1}^{m+n} X_j = b-a\right) \\ &= P(S_{m+n} = b \mid S_m = a). \quad \square \end{aligned}$$

Remark 10.4.5. The sum $\sum_{i=m+1}^{m+n} X_i$ is independent of the first m partial sums $S_0, \ldots, S_m$. This is an essential observation for the proof below.

Proposition 10.4.6. *S_n has the Markov property; that is,*

$$P(S_{m+n} = b \mid S_m = s_m, \ldots, S_0 = s_0) = P(S_{m+n} = b \mid S_m = s_m).$$

Proof.

$$\begin{aligned} &P(S_{m+n} = b \mid S_m = s_m, \ldots, S_0 = s_0) \\ &\qquad = \frac{P(\sum_{i=1}^{m+n} X_i + S_0 = b, S_m = s_m, \ldots, S_0 = s_0)}{P(S_m = s_m, \ldots, S_0 = s_0)} \\ &\qquad = \frac{P(\sum_{i=m+1}^{m+n} X_i = b - s_m, S_m = s_m, \ldots, S_0 = s_0)}{P(S_m = s_m, \ldots, S_0 = s_0)} \\ &\qquad = \frac{P(\sum_{i=m+1}^{m+n} X_i = b - s_m) P(S_m = s_m, \ldots, S_0 = s_0)}{P(S_m = s_m, \ldots, S_0 = s_0)} \\ &\qquad = P(\textstyle\sum_{i=m+1}^{m+n} X_i = b - s_m) = P(S_{m+n} = b \mid S_m = s_m). \quad \square \end{aligned}$$

10.4.2 Gambler's Ruin

Random walks can have absorbing barriers where once you get too far in one direction of the other, you are stuck there forever. This is the mathematical equivalent of bowling a gutter ball.

We consider the case of a gambler who plays a repeated game against the house until either he wins all the money or the house wins all the money. Assume he starts with k dollars and that there are N total dollars between him and the house. With each game, he wins a dollar with probability p or loses one with probability $q = 1 - p$. Thus we have that $S_0 = k$, and that the game terminates when the gambler is ruined, that is, when $S_n = 0$ or when the house is ruined, that is, $S_n = N$.

Let y_k be the probability that the gambler gets ruined if he starts with k dollars. Obviously, $y_0 = 1$ and $y_N = 0$; these are the boundary conditions for the system. For $1 \leq k \leq N-1$, we have that

$$y_k = py_{k+1} + qy_{k-1}. \tag{10.11}$$

This is called a *difference equation*, specifically a second-order difference equation since the next state y_{k+1} can be written as a sum of the two previous states y_k and y_{k-1}, respectively. This can be written as a matrix equation

$$\begin{pmatrix} y_{k+1} \\ y_k \end{pmatrix} = \underbrace{\begin{pmatrix} 1/p & -q/p \\ 1 & 0 \end{pmatrix}}_{A} \begin{pmatrix} y_k \\ y_{k-1} \end{pmatrix}.$$

Thus, we have that

$$\begin{pmatrix} y_{k+1} \\ y_k \end{pmatrix} = \begin{pmatrix} 1/p & -q/p \\ 1 & 0 \end{pmatrix}^k \begin{pmatrix} y_1 \\ y_0 \end{pmatrix}.$$

It is well known that the solution of a linear difference equation of this form can be written $y_k = a\lambda_1^k + b\lambda_2^k$, when the eigenvalues λ_1 and λ_2 of A are distinct, and $y_k = ak\lambda^{k-1} + b\lambda^k$ when $\lambda_1 = \lambda_2 = \lambda$. In either case, a and b are constants determined by the boundary conditions.

We compute the eigenvalues of A by finding the roots of the characteristic polynomial.

$$p\lambda^2 - \lambda + q.$$

The roots satisfy

$$\lambda = \frac{1 \pm \sqrt{1-4pq}}{2p} = \frac{1 \pm |1-2p|}{2p} = \left\{ \frac{q}{p}, 1 \right\}.$$

These are the same when $p = q = 1/2$ and are distinct otherwise. In other words,, we have

$$y_k = \begin{cases} a\left(\dfrac{q}{p}\right)^k + b & p \neq \dfrac{1}{2} \\[2ex] ak + b & p = \dfrac{1}{2}. \end{cases}$$

Inserting the boundary conditions, we get that

$$0 = y_N = \begin{cases} a\left(\dfrac{q}{p}\right)^N + b & p \neq \dfrac{1}{2} \\[2ex] aN + b & p = \dfrac{1}{2} \end{cases}$$

and

$$1 = y_0 = \begin{cases} a+b & p \neq \dfrac{1}{2} \\ \\ b & p = \dfrac{1}{2}. \end{cases}$$

Thus, we have that

$$y_k = \begin{cases} \dfrac{\left(\dfrac{q}{p}\right)^k - \left(\dfrac{q}{p}\right)^N}{1 - \left(\dfrac{q}{p}\right)^N} & p \neq \dfrac{1}{2} \\ \\ 1 - \dfrac{k}{N} & p = \dfrac{1}{2}. \end{cases} \tag{10.12}$$

Remark 10.4.7. One can show that in the limit as $p, q \to 1/2$, the $p \neq 1/2$ case in (10.12) converges to the $p = 1/2$ case; see Exercise 10.20.

Remark 10.4.8. If $q \geq p$ and $N \to \infty$, then $y_k \to 1$, regardless of the size of k. This means that as the size of the house's initial stake gets large, the probability that the house will ruin the gambler approaches 1.

10.4.3 Reflecting Barriers

Suppose that the gambler has a rich uncle who owns the casino gives him a dollar every time he's ruined (taking a dollar from the house so that the total dollars is N. TODO.

Exercises

Note to the student: Each section of this chapter has several corresponding exercises, all collected here at the end of the chapter. The exercises between the first and second line are for Section 1, the exercises between the second and third lines are for Section 2, and so forth.

You should **work every exercise** (your instructor may choose to let you skip some of the advanced exercises marked with *). We have carefully selected them, and each is important for your ability to understand subsequent material. Many of the examples and results proved in the exercises are used again later in the text. Exercises marked with ⚠ are especially important and are likely to be used later in this book and beyond. Those marked with † are harder than average, but should still be done.

Although they are gathered together at the end of the chapter, we strongly recommend you do the exercises for each section as soon as you have completed the section, rather than saving them until you have finished the entire chapter.

10.1. Suppose that on any given day the weather is either rainy or sunny. If today is rainy, tomorrow will also be rainy with probability p and sunny with probability $1-p$. Similarly, if today is sunny, tomorrow will also be sunny with probability r and rainy with probability $1-r$.

(i) Construct a Markov chain to model this situation.

(ii) Write the transition matrix for this Markov chain.

(iii) Draw the transition diagram for this Markov chain.

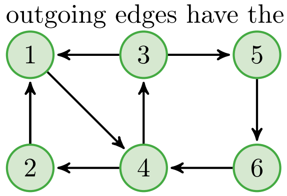
10.2. Building on the previous problem (Exercise 10.1), suppose now that the weather tomorrow depends on the weather of the past two days. If the weather has been sunny for two days, it will be rainy tomorrow with probability 1, and if it has been rainy for two days it will be sunny with probability 1. Otherwise, the transitions are the same as in the previous problem.

(i) Model this situation with a Markov chain. Hint: Consider enlarging the state space.

(ii) Construct the transition matrix

(iii) Draw the transition diagram.

10.3. Assume that for every vertex in the following transition diagram, all the outgoing edges have the same probability.



For the Markov chain $(X_t)_{t\in\mathbb{N}}$ with this transition diagram

(i) Find the conditional probability $P(X_2 = 1 \mid X_1 = 3)$.

(ii) Write the transition matrix for this Markov chain.

(iii) Find the conditional probability $P(X_2 = 1 \mid X_0 = 4)$.

(iv) If initially every state is equally likely ($P(X_0 = k) = \frac{1}{6}$ for all $k \in \{1, \dots, 6\}$), then find the marginal probability that $X_2 = 1$.

(v) If initially every state is equally likely, find the marginal probability distribution for X_{10^n} (find the vector $(P(X_{10^n} = 1), \dots, P(X_{10^n} = 6))$) for every $n \in \{0, 1, 2, 3, 4, 5\}$.

10.4. A (real-valued) nonnegative square matrix is *column stochastic* if the entries in each column sum to 1.

(i) Prove that a nonnegative square matrix is column stochastic if and only if it has an eigenvalue equal to 1 and a corresponding left (row) eigenvector equal to $\mathbb{1}^{\mathsf{T}} = \begin{bmatrix} 1 & \dots & 1 \end{bmatrix}$.

(ii) For any column-stochastic matrix Q and any $k \in \mathbb{N}$, prove that Q^k is also column stochastic.

(iii) Recall (Volume 1, Lemma 12.3.13) that the spectral radius $r(A)$ of a square matrix A is $\lim_{k\to\infty} \|A^k\|^{1/k}$ for any matrix norm $\|\cdot\|$. Moreover, $r(A) = \sup_{\lambda\in\sigma(A)} |\lambda|$ is the largest modulus of any eigenvalue of A (Volume 1, Cor. 12.4.7). Use the 1-norm and the previous results to show that the spectral radius of any column-stochastic matrix is 1, and hence all its eigenvalues lie in the unit disk $\{z \in \mathbb{C} : |z| \leq 1\}$.

10.5. Prove Corollary 10.1.17.

10.6. Prove Proposition 10.1.21.

10.7.* Prove Proposition 10.1.27.

10.8. Prove Proposition 10.2.4.

10.9. Finish the proof of Proposition 10.2.6 by proving that when starting at a transient state k, there is a nonzero chance of never returning to k.

10.10. Prove Proposition 10.2.11.

10.11. A professor has m probability books, which she keeps in a pile. Occasionally, she picks one book out, independent of past choices, and after using it, puts it on top of the pile. The probability of choosing a book is not determined by its location in the pile, but rather by the book itself—some books are more useful than others. Assume that the probability of choosing book number i is β_i and $\beta_i > 0$ for all i. Show that the stationary probability that this book is on the top of the pile is also β_i.

10.12. A traffic survey on a particular road finds that three out of every four trucks on the road are followed by a car, while only one out of every five cars is followed by a truck.

(i) Describe a Markov chain that models this situation.

(ii) Find the stationary distribution for this Markov chain. Hint: The stationary distribution is an eigenvector, which isn't difficult to compute in this 2×2 case.

(iii) Interpret the meaning of the stationary distribution in terms of percentages of cars and trucks on the road.

10.13. Consider the $n \times n$ column-stochastic matrix Q of the form

$$Q = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \ddots & 1 \\ 1 & 0 & 0 & \dots & 0 \end{bmatrix}.$$

(i) Prove that the eigenvalues of Q are the nth roots of unity.

(ii) Prove that the stationary distribution for Q is $(\frac{1}{n}, \dots, \frac{1}{n})$.

(iii) But starting with an initial distribution $\mathbf{x} = (1, 0, 0, \cdots, 0)$, show the sequence $(Q^k\mathbf{x})_{k=0}^{\infty}$ does not converge. Why doesn't this contradict the theorem on the power method?

10.14. Finish the proof of Theorem 10.3.8 by proving that any finite-state, primitive Markov chain is aperiodic.

10.15. Prove Corollary 10.3.10.

10.16. Let Q be the transition matrix of an irreducible Markov chain with stationary distribution $\boldsymbol{\pi}$. Let W be the matrix with each column equal $\boldsymbol{\pi}$. Show that

$$(I + Q + \cdots + Q^{n-1})(I - Q + W) = I - Q^n + nW,$$

and from this show that

$$\frac{1}{n}(I + Q + \cdots + Q^{n-1}) \to W$$

as $n \to \infty$. This gives an alternative (not necessarily more efficient) to the power method for computing the stationary distribution. Hint: Prove that the matrix $(I - Q + W)$ is invertible, either using spectral decomposition (Volume 1, Theorem 12.6.12) or argue that if $\mathbf{x}^{\mathsf{T}}(I - Q + W) = 0$, then $\mathbf{x}^{\mathsf{T}} = 0$. Also show that $W(I - Q + W) = W$, so $W(I - Q + W)^{-1} = W$.

10.17. A random knight (on a chessboard) makes each permissible move with equal probability. If it starts in a corner, how long on average will it take to return? Hint: Example 10.3.15 could be helpful.

10.18.* Write the transition matrix for the gambler's ruin problem in the case that $N = 3$.

10.19.* Prove the claim in Remark 10.4.7 that as $p, q \to 1/2$, the $p \neq 1/2$ case in (10.12) converges to the $p = 1/2$ case.

Notes