3

MARKOV CHAINS FOR THE LONG TERM

There exists everywhere a medium in things, determined by equilibrium.

—Dmitri Mendeleev

3.1 LIMITING DISTRIBUTION

In many cases, a Markov chain exhibits a long-term limiting behavior. The chain settles down to an equilibrium distribution, which is independent of its initial state.

Limiting Distribution

Let $X_0, X_1, \ldots$ be a Markov chain with transition matrix $\boldsymbol{P}$. A *limiting distribution* for the Markov chain is a probability distribution $\boldsymbol{\lambda}$ with the property that for all i and j,

$$\lim_{n\to\infty} P^n_{ij} = \lambda_j.$$

The definition of limiting distribution is equivalent to each of the following:

(i) For any initial distribution, and for all j,

$$\lim_{n\to\infty} P(X_n = j) = \lambda_j.$$

Introduction to Stochastic Processes with R, First Edition. Robert P. Dobrow.

(ii) For any initial distribution $\boldsymbol{\alpha}$,

$$\lim_{n\to\infty} \boldsymbol{\alpha P}^n = \boldsymbol{\lambda}.$$

(iii)

$$\lim_{n\to\infty} \boldsymbol{P}^n = \boldsymbol{\Lambda},$$

where $\boldsymbol{\Lambda}$ is a stochastic matrix all of whose rows are equal to $\boldsymbol{\lambda}$.

We interpret λ_j as the long-term probability that the chain hits state j. By the uniqueness of limits, if a Markov chain has a limiting distribution, then that distribution is unique.

If a limiting distribution exists, a *quick and dirty* numerical method to find it is to take high matrix powers of the transition matrix until one obtains an obvious limiting matrix with equal rows. The common row is the limiting distribution. Examples of this approach have been given in Section 2.5.

Numerical methods, however, have their limits (no pun intended), and the emphasis in this chapter is on exact solutions and theoretical results.

For the general two-state Markov chain, matrix powers can be found exactly in order to compute the limiting distribution.

Example 3.1 (Two-state Markov chain) The transition matrix for a general two-state chain is

$$\boldsymbol{P} = \begin{array}{c c} & \begin{array}{cc} 1 & 2 \end{array} \\ \begin{array}{c} 1 \\ 2 \end{array} & \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix} \end{array},$$

for $0 \le p, q \le 1$. If $p + q = 1$,

$$\boldsymbol{P} = \begin{pmatrix} 1-p & p \\ 1-p & p \end{pmatrix},$$

and $\boldsymbol{P}^n = \boldsymbol{P}$ for all $n \ge 1$. Thus, $\boldsymbol{\lambda} = (1-p, p)$ is the limiting distribution.

Assume $p + q \ne 1$. To find $\boldsymbol{P}^n$, consider the entry P^n_{11}. As $\boldsymbol{P}^n = \boldsymbol{P}^{n-1}\boldsymbol{P}$,

$$\begin{aligned} P^n_{11} &= (P^{n-1}P)_{11} = P^{n-1}_{11} P_{11} + P^{n-1}_{12} P_{21} \\ &= P^{n-1}_{11}(1-p) + P^{n-1}_{12} q \\ &= P^{n-1}_{11}(1-p) + \left(1 - P^{n-1}_{11}\right) q \\ &= q + (1-p-q)P^{n-1}_{11} \quad ,\text{for} \quad n \ge 1. \end{aligned}$$

The next-to-last equality uses the fact that $P_{11}^{n-1} + P_{12}^{n-1} = 1$, since $\boldsymbol{P}^{n-1}$ is a stochastic matrix. Unwinding the recurrence gives

$$\begin{aligned}
P_{11}^{n} &= q + (1-p-q)P_{11}^{n-1} \\
&= q + q(1-p-q) + (1-p-q)^2 P_{11}^{n-2} \\
&= q + q(1-p-q) + q(1-p-q)^2 + (1-p-q)^3 P_{11}^{n-3} \\
&= \cdots = q\sum_{k=0}^{n-1}(1-p-q)^k + (1-p-q)^n \\
&= (1-p-q)^n + q\frac{1-(1-p-q)^n}{1-(1-p-q)} \\
&= \frac{q}{p+q} + \frac{p}{p+q}(1-p-q)^n.
\end{aligned}$$

The matrix entry

$$P_{22}^{n} = \frac{p}{p+q} + \frac{q}{p+q}(1-p-q)^n$$

is found similarly. Since the rows of $\boldsymbol{P}^n$ sum to 1,

$$\boldsymbol{P}^n = \frac{1}{p+q}\begin{pmatrix} q + p(1-p-q)^n & p - p(1-p-q)^n \\ q - q(1-p-q)^n & p + q(1-p-q)^n \end{pmatrix}. \tag{3.1}$$

If p and q are not both 0, nor both 1, then $|1-p-q| < 1$ and

$$\lim_{n\to\infty} \boldsymbol{P}^n = \frac{1}{p+q}\begin{pmatrix} q & p \\ q & p \end{pmatrix}.$$

The limiting distribution is

$$\lambda = \left(\frac{q}{p+q}, \frac{p}{p+q}\right).$$

Observe that in addition to giving the limiting distribution, Equation (3.1) reveals the rate of convergence to that limit. The convergence is exponential and governed by the quantity $(1-p-q)^n$. ■

Proportion of Time in Each State

The limiting distribution gives the long-term probability that a Markov chain hits each state. It can also be interpreted as the long-term proportion of time that the chain visits each state. To make this precise, let $X_0, X_1, \ldots$ be a Markov chain with transition matrix $\boldsymbol{P}$ and limiting distribution λ. For state j, define indicator random variables

$$I_k = \begin{cases} 1, & \text{if } X_k = j, \\ 0, & \text{otherwise,} \end{cases}$$

for $k = 0, 1, \ldots$ Then, $\sum_{k=0}^{n-1} I_k$ is the number of times the chain visits j in the first n steps (counting X_0 as the first step). From initial state i, the long-term expected proportion of time that the chain visits j is

$$\begin{aligned}\lim_{n\to\infty} E\left(\frac{1}{n}\sum_{k=0}^{n-1} I_k|X_0 = i\right) &= \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} E(I_k|X_0 = i) \\ &= \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} P(X_k = j|X_0 = i) \\ &= \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} P_{ij}^k \\ &= \lim_{n\to\infty} P_{ij}^n = \lambda_j.\end{aligned}$$

The next-to-last equality applies a result in analysis known as Cesaro's lemma. The lemma states that if a sequence of numbers converges to a limit, then the sequence of partial averages also converges to that limit. That is, if $x_n \to x$, as $n \to \infty$, then $(x_1 + \cdots + x_n)/n \to x$, as $n \to \infty$.

Example 3.2 After work, Angel goes to the gym and either does aerobics, weights, yoga, or gets a massage. Each day, Angel decides her workout routine based on what she did the previous day according to the Markov transition matrix

$$\boldsymbol{P} = \begin{array}{l} \\ \text{Aerobics} \\ \text{Massage} \\ \text{Weights} \\ \text{Yoga} \end{array} \begin{array}{c} \begin{array}{cccc} \text{Aerobics} & \text{Massage} & \text{Weights} & \text{Yoga} \end{array} \\ \begin{pmatrix} 0.1 & 0.2 & 0.4 & 0.3 \\ 0.4 & 0.0 & 0.4 & 0.2 \\ 0.3 & 0.3 & 0.0 & 0.4 \\ 0.2 & 0.1 & 0.4 & 0.3 \end{pmatrix} \end{array}.$$

Taking high matrix powers gives the limiting distribution

Aerobics	Massage	Weight	Yoga
0.238	0.164	0.286	0.312

See the following `R` code, where Angel's gym visits are simulated for 100 days. During that time, Angel did aerobics on 26 days, got a massage 14 times, did weights on 31 days, and did yoga 29 times. The proportion of visits to each state is

Aerobics	Massage	Weighs	Yoga
0.26	0.14	0.31	0.29

These proportions are relatively close to the actual limiting distribution of the chain notwithstanding the fact that the estimates are based on just 100 steps. Compare the results to the million step simulation, also given in the R code. ■

R: Angel at the Gym

```
# gym.R
> P
         Aerobics Massage Weights Yoga
Aerobics      0.1     0.2     0.4  0.3
Massage       0.4     0.0     0.4  0.2
Weights       0.3     0.3     0.0  0.4
Yoga          0.2     0.1     0.4  0.3
> init <- c(1/4,1/4,1/4,1/4) # initial distribution
> states <- c("a","m","w","y")
# simulate Markov chain for 100 steps
> simlist <- markov(init,P,100,states)
> mwyaaywyayawyayawymwywamwawyawywywyywywyawyamwaway
> amamawywmyawawmawywmwywmwmyaywaywywamwyyymwawamaay
> table(simlist)/100
Aerobics  Massage  Weights     Yoga
  0.26     0.14      0.31      0.29
> steps <- 1000000  # one million steps
> simlist <- markov(init,P,steps,states)
> table(simlist)/steps
Aerobics  Massage  Weights     Yoga
0.237425 0.164388 0.285548 0.312640
```

3.2 STATIONARY DISTRIBUTION

It is interesting to consider what happens if we assign the limiting distribution of a Markov chain to be the initial distribution of the chain.

For the two-state chain, as in Example 3.1, the limiting distribution is

$$\lambda = \left(\frac{q}{p+q}, \frac{p}{p+q} \right).$$

Let λ be the initial distribution for such a chain. Then, the distribution of X_1 is

$$\begin{aligned}
\lambda \boldsymbol{P} &= \left(\frac{q}{p+q}, \frac{p}{p+q} \right) \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix} \\
&= \left(\frac{q(1-p)+pq}{p+q}, \frac{qp+p(1-q)}{p+q} \right)
\end{aligned}$$

$$= \left(\frac{q}{p+q}, \frac{p}{p+q}\right) = \lambda.$$

That is, $\boldsymbol{\lambda P} = \boldsymbol{\lambda}$. A probability vector $\boldsymbol{\pi}$ that satisfies $\boldsymbol{\pi}\mathbf{P} = \boldsymbol{\pi}$ plays a special role for Markov chains.

Stationary Distribution

Let $X_0, X_1, \ldots$ be a Markov chain with transition matrix $\boldsymbol{P}$. A *stationary distribution* is a probability distribution $\boldsymbol{\pi}$, which satisfies

$$\boldsymbol{\pi} = \boldsymbol{\pi P}. \tag{3.2}$$

That is,

$$\pi_j = \sum_i \pi_i P_{ij}, \quad \text{for all } j.$$

If we assume that a stationary distribution $\boldsymbol{\pi}$ is the initial distribution, then Equation (3.2) says that the distribution of X_0 is the same as the distribution of X_1. Since the chain started at $n = 1$ is also a Markov chain with transition matrix $\boldsymbol{P}$, it follows that X_2 has the same distribution as X_1. In fact, all of the X_n have the same distribution, as

$$\boldsymbol{\pi P}^n = (\boldsymbol{\pi P})\boldsymbol{P}^{n-1} = \boldsymbol{\pi P}^{n-1} = (\boldsymbol{\pi P})\boldsymbol{P}^{n-2} = \boldsymbol{\pi P}^{n-2} = \cdots = \boldsymbol{\pi P} = \boldsymbol{\pi}.$$

If the initial distribution is a stationary distribution, then $X_0, X_1, X_2, \ldots$ is a sequence of identically distributed random variables.

The name *stationary* comes from the fact that if the chain starts in its stationary distribution, then it stays in that distribution. We refer to the *stationary Markov chain* or the Markov chain *in stationarity* for the chain started in its stationary distribution.

If $X_0, X_1, X_2, \ldots$ is a stationary Markov chain, then for any $n > 0$, the sequence $X_n, X_{n+1}, X_{n+2}, \ldots$ is also a stationary Markov chain with the same transition matrix and stationary distribution as the original chain.

(The fact that the stationary chain is a sequence of identically distributed random variables does not mean that the random variables are independent. On the contrary, the dependency structure between successive random variables in a Markov chain is governed by the transition matrix, regardless of the initial distribution.)

Other names for the stationary distribution are *invariant*, *steady-state*, and *equilibrium* distribution. The latter highlights the fact that there is an intimate connection between the stationary distribution and the limiting distribution. If a Markov chain has a limiting distribution then that distribution is a stationary distribution.

Limiting Distributions are Stationary Distributions

Lemma 3.1. *Assume that $\boldsymbol{\pi}$ is the limiting distribution of a Markov chain with transition matrix $\boldsymbol{P}$. Then, $\boldsymbol{\pi}$ is a stationary distribution.*

Proof. Assume that $\boldsymbol{\pi}$ is the limiting distribution. We need to show that $\boldsymbol{\pi P} = \boldsymbol{\pi}$. For any initial distribution $\boldsymbol{\alpha}$,

$$\boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\alpha P}^n = \lim_{n\to\infty} \boldsymbol{\alpha}(\boldsymbol{P}^{n-1}\boldsymbol{P}) = \left(\lim_{n\to\infty} \boldsymbol{\alpha P}^{n-1}\right)\boldsymbol{P} = \boldsymbol{\pi P},$$

which uses the fact that if $\lim_{n\to\infty} x_n = x$, then $\lim_{n\to\infty} x_{n-1} = x$. ■

Unfortunately, the converse of Lemma 3.1 is not true—stationary distributions are not necessarily limiting distributions. For a counterexample, take the Markov chain with transition matrix

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

Solving $\boldsymbol{\pi P} = \boldsymbol{\pi}$, or

$$\left(\pi_1, \pi_2\right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \left(\pi_1, \pi_2\right),$$

gives $\pi_1 = \pi_2$. Since the stationary distribution is a probability vector, the unique solution is $\boldsymbol{\pi} = (1/2, 1/2)$. The stationary distribution is uniform on each state. However, the chain has no limiting distribution. The process evolves by flip-flopping back and forth between states. As in the case of random walk on a cycle with an even number of vertices, the position of the walk after n steps depends on the starting vertex and the parity of n.

Another counterexample is the Markov chain with transition matrix

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

This process is rather boring—the chain simply stays forever in its starting state. The chain has no limiting distribution, as the long-term state of the chain depends upon the starting state. However, *every* probability vector is a stationary distribution since $\boldsymbol{xP} = \boldsymbol{x}$, for all vectors $\boldsymbol{x}$.

Thus, there are Markov chains with more than one stationary distribution; there are Markov chains with unique stationary distributions that are not limiting distributions; and there are even Markov chains that do not have stationary distributions.

However, a large and important class of Markov chains has unique stationary distributions that are the limiting distribution of the chain. A goal of this chapter is to characterize such chains.

Regular Matrices

A matrix $\boldsymbol{M}$ is said to be *positive* if all the entries of $\boldsymbol{M}$ are positive. We write $\boldsymbol{M} > 0$. Similarly, write $\boldsymbol{x} > 0$ for a vector $\boldsymbol{x}$ with all positive entries.

Regular Transition Matrix

A transition matrix $\boldsymbol{P}$ is said to be *regular* if some power of $\boldsymbol{P}$ is positive. That is, $\boldsymbol{P}^n > 0$, for some $n \geq 1$.

For example,

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1 & 0 & 0 \\ 1/2 & 1/2 & 0 \end{pmatrix}$$

is regular, since

$$\boldsymbol{P}^4 = \begin{pmatrix} 9/16 & 5/16 & 1/8 \\ 1/4 & 3/8 & 3/8 \\ 1/2 & 5/16 & 3/16 \end{pmatrix}$$

is positive. However,

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

is not regular, since the powers of $\boldsymbol{P}$ cycle through the matrices

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{P}^2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \text{and } \boldsymbol{P}^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

If the transition matrix of a Markov chain is regular, then the chain has a limiting distribution, which is the unique stationary distribution of the chain.

Limit Theorem for Regular Markov Chains

Theorem 3.2. *A Markov chain whose transition matrix* $\boldsymbol{P}$ *is regular has a limiting distribution, which is the unique, positive, stationary distribution of the chain. That is, there exists a unique probability vector* $\boldsymbol{\pi} > 0$, *such that*

$$\lim_{n\to\infty} P_{ij}^n = \pi_j,$$

for all i, j, *where*

$$\sum_i \pi_i P_{ij} = \pi_j.$$

Equivalently, there exists a positive stochastic matrix $\boldsymbol{\Pi}$ *such that*

$$\lim_{n\to\infty} \boldsymbol{P}^n = \boldsymbol{\Pi},$$

where $\mathbf{\Pi}$ *has equal rows with common row* $\boldsymbol{\pi}$*, and* $\boldsymbol{\pi}$ *is the unique probability vector, which satisfies*

$$\boldsymbol{\pi}\boldsymbol{P} = \boldsymbol{\pi}.$$

The proof of Theorem 3.2 is deferred to Section 3.10.

Example 3.3 Assume that a Markov chain has transition matrix

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1-p & p \\ p & 0 & 1-p \\ 1-p & p & 0 \end{pmatrix},$$

for $0 < p < 1$. Find the limiting distribution.

Solution We find that

$$\boldsymbol{P}^2 = \begin{pmatrix} 2p(1-p) & p^2 & (1-p)^2 \\ (1-p)^2 & 2p(1-p) & p^2 \\ p^2 & (1-p)^2 & 2p(1-p) \end{pmatrix}.$$

Since $0 < p < 1$, the matrix $\boldsymbol{P}^2$ is positive. Thus, $\boldsymbol{P}$ is regular. By Theorem 3.2, the limiting distribution is the stationary distribution.

How to find the stationary distribution of a Markov chain is the topic of the next section. However, for now we give the reader a little help and urge them to try $\boldsymbol{\pi} = (1/3, 1/3, 1/3)$.

Indeed, $\boldsymbol{\pi}\boldsymbol{P} = \boldsymbol{\pi}$, as

$$\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right) \begin{pmatrix} 0 & 1-p & p \\ p & 0 & 1-p \\ 1-p & p & 0 \end{pmatrix} = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right).$$

The uniform distribution $\boldsymbol{\pi}$ is the unique stationary distribution of the chain, and thus the desired limiting distribution.

The example is interesting because the limiting distribution is uniform for *all* choices of $0 < p < 1$. ■

Here is one way to tell if a stochastic matrix is not regular. If for some power n, all the 0s in $\boldsymbol{P}^n$ appear in the same locations as all the 0s in $\boldsymbol{P}^{n+1}$, then they will appear in the same locations for all higher powers, and the matrix is not regular.

Example 3.4 A Markov chain has transition matrix

$$\boldsymbol{P} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ \frac{1}{4} & 0 & 0 & \frac{1}{2} & \frac{1}{4} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{2} & 0 & 0 & \frac{1}{4} \end{pmatrix}.$$

Determine if the matrix is regular.

Solution We find that

$$\boldsymbol{P}^4 = \begin{pmatrix} \frac{9}{64} & \frac{7}{32} & \frac{1}{8} & \frac{3}{16} & \frac{21}{64} \\ \frac{21}{256} & \frac{11}{128} & \frac{15}{32} & \frac{11}{64} & \frac{49}{256} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{15}{16} & \frac{1}{16} & 0 \\ \frac{35}{256} & \frac{21}{128} & \frac{7}{32} & \frac{13}{64} & \frac{71}{256} \end{pmatrix} \text{ and } \boldsymbol{P}^5 = \begin{pmatrix} \frac{35}{256} & \frac{21}{128} & \frac{7}{32} & \frac{13}{64} & \frac{71}{256} \\ \frac{71}{1024} & \frac{49}{512} & \frac{71}{128} & \frac{33}{256} & \frac{155}{1024} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{31}{32} & \frac{1}{32} & 0 \\ \frac{113}{1024} & \frac{71}{512} & \frac{41}{128} & \frac{47}{256} & \frac{253}{1024} \end{pmatrix}.$$

Since the 0s are in the same locations for both matrices, we conclude that $\boldsymbol{P}$ is not regular. ∎

Finding the Stationary Distribution

Assume that $\boldsymbol{\pi}$ is a stationary distribution for a Markov chain with transition matrix $\boldsymbol{P}$. Then,

$$\sum_i \pi_i P_{ij} = \pi_j, \text{ for all states } j,$$

which gives a system of linear equations. If $\boldsymbol{P}$ is a $k \times k$ matrix, the system has k equations and k unknowns. Since the rows of $\boldsymbol{P}$ sum to 1, the $k \times k$ system will contain a redundant equation.

For the general two-state chain, with

$$\boldsymbol{P} = \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix},$$

the equations are

$$(1-p)\pi_1 + q\pi_2 = \pi_1$$
$$p\pi_1 + (1-q)\pi_2 = \pi_2.$$

The equations are redundant and lead to $\pi_1 p = \pi_2 q$. If p and q are not both zero, then together with the condition $\pi_1 + \pi_2 = 1$, the unique solution is

$$\boldsymbol{\pi} = \left(\frac{q}{p+q}, \frac{p}{p+q} \right).$$

Example 3.5 Find the stationary distribution of the weather Markov chain of Example 2.3, with transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ \text{Rain} \\ \text{Snow} \\ \text{Clear} \end{array} \begin{array}{c} \begin{array}{ccc} \text{Rain} & \text{Snow} & \text{Clear} \end{array} \\ \begin{pmatrix} 1/5 & 3/5 & 1/5 \\ 1/10 & 4/5 & 1/10 \\ 1/10 & 3/5 & 3/10 \end{pmatrix} \end{array}.$$

Solution The linear system to solve is

$$\begin{aligned}
(1/5)\pi_1 + (1/10)\pi_2 + (1/10)\pi_3 &= \pi_1 \\
(3/5)\pi_1 + (4/5)\pi_2 + (3/5)\pi_3 &= \pi_2 \\
(1/5)\pi_1 + (1/10)\pi_2 + (3/10)\pi_3 &= \pi_3 \\
\pi_1 + \pi_2 + \pi_3 &= 1.
\end{aligned}$$

One of the first three equations is redundant. The unique solution is

$$\boldsymbol{\pi} = \left(\frac{1}{9}, \frac{3}{4}, \frac{5}{36} \right).$$

■

`R` : Finding the Stationary Distribution

The `R` function `stationary(P)` finds the stationary distribution of a Markov chain with transition matrix `P`. The function is contained in the **utilities.R** file.

```
> P
       Rain Snow Clear
Rain    0.2  0.6   0.2
Snow    0.1  0.8   0.1
Clear   0.1  0.6   0.3
> stationary(P)
[1] 0.1111 0.7500 0.1389
# check that this is a stationary distribution
> stationary(P) %*% P
         Rain    Snow    Clear
[1]    0.1111    0.75   0.1389
```

Here is a useful technique for finding the stationary distribution, which reduces by one the number of equations to solve. It makes use of the fact that if $\boldsymbol{x}$ is a vector, not necessarily a probability vector, which satisfies $\boldsymbol{xP} = \boldsymbol{x}$, then $(c\boldsymbol{x})\boldsymbol{P} = c\boldsymbol{x}$, for all constants c. It follows that if one can find a non-negative $\boldsymbol{x}$, which satisfies $\boldsymbol{xP} = \boldsymbol{x}$, then a unique probability vector solution $\boldsymbol{\pi} = c\boldsymbol{x}$ can be gotten by an appropriate choice of c so that the rows of $c\boldsymbol{x}$ sum to 1. In particular, let $c = 1/\sum_j x_j$, the reciprocal of the sum of the components of $\boldsymbol{x}$.

The linear system $\sum_i \pi_i P_{ij} = \pi_j$, without the constraint $\sum_i \pi_i = 1$, has one redundant equation. Our solution method consists of (i) eliminating a redundant equation and (ii) solving the resulting system for $\boldsymbol{x} = (1, x_2, x_3, \ldots)$, where the first (or any) component of $\boldsymbol{x}$ is replaced by 1.

For a Markov chain with k states, this method reduces the problem to solving a $(k-1) \times (k-1)$ linear system. If the original chain has a unique stationary distribution, then the reduced linear system will have a unique solution, but one which is not necessarily a probability vector. To make it a probability vector whose components sum to 1, divide by the sum of the components. In other words, the unique stationary distribution is

$$\boldsymbol{\pi} = \frac{1}{1 + x_2 + \cdots + x_k}(1, x_2, \ldots, x_k).$$

To illustrate the method, consider the transition matrix

$$\boldsymbol{P} = \begin{pmatrix} 1/3 & 1/2 & 1/6 \\ 1/2 & 1/2 & 0 \\ 1/4 & 1/2 & 1/4 \end{pmatrix}.$$

To find the stationary distribution, first let $\boldsymbol{x} = (1, x_2, x_3)$. Then, $\boldsymbol{xP} = \boldsymbol{x}$ gives a 3×3 linear system. The first two equations are

$$(1/3)(1) + (1/2)x_2 + (1/4)x_3 = 1,$$
$$(1/2)(1) + (1/2)x_2 + (1/2)x_3 = x_2,$$

or

$$(1/2)x_2 + (1/4)x_3 = 2/3,$$
$$(-1/2)x_2 + (1/2)x_3 = -1/2,$$

with unique solution $\boldsymbol{x} = (1, 11/9, 2/9)$. The sum of the components is

$$1 + \frac{11}{9} + \frac{2}{9} = \frac{22}{9}.$$

The stationary distribution is

$$\boldsymbol{\pi} = \frac{9}{22}\left(1, \frac{11}{9}, \frac{2}{9}\right) = \left(\frac{9}{22}, \frac{11}{22}, \frac{2}{22}\right).$$

Example 3.6 A Markov chain on $\{1,2,3,4\}$ has transition matrix

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

for $0 < p < 1$. Find the stationary distribution.

Solution Let $\boldsymbol{x} = (x_1, x_2, x_3, x_4)$, with $x_1 = 1$. Take

$$x_j = \sum_{i=1}^{4} x_i P_{ij},$$

for $j = 1, 2$, and 4. This gives

$$\begin{aligned} p + \left(\frac{1-p}{2}\right) x_2 \qquad\qquad\qquad\qquad &= 1, \\ 1 - p + \qquad px_2 + \left(\frac{1-p}{2}\right) x_3 \qquad &= x_2, \\ \left(\frac{1-p}{2}\right) x_3 + px_4 &= x_4, \end{aligned}$$

with solution $x_2 = x_3 = 2$ and $x_1 = x_4 = 1$. The stationary distribution is

$$\boldsymbol{\pi} = \frac{1}{1+2+2+1}\left(1,2,2,1\right) = \left(\frac{1}{6}, \frac{2}{6}, \frac{2}{6}, \frac{1}{6}\right).$$

■

Example 3.7 (The Ehrenfest dog–flea model) The Ehrenfest dog–flea model was originally proposed by physicists Tatyana and Paul Ehrenfest to describe the diffusion of gases. Mathematician Mark Kac called it "one of the most instructive models in the whole of physics."

Two dogs—Lisa and Cooper—share a population of N fleas. At each discrete unit of time, one of the fleas jumps from the dog it is on to the other dog. Let X_n denote the number of fleas on Lisa after n jumps. If there are i fleas on Lisa, then on the next jump the number of fleas on Lisa either goes up by one, if one of the $N - i$ fleas on Cooper jumps to Lisa, or goes down by one, if one of the i fleas on Lisa jumps to Cooper.

The process is a Markov chain on $\{0, 1, \ldots, N\}$, with transition matrix

$$P_{ij} = \begin{cases} i/N, & \text{if } \quad j = i-1, \\ (N-i)/N, & \text{if } \quad j = i+1, \\ 0, & \text{otherwise.} \end{cases}$$

Here is the Ehrenfest transition matrix for $N = 5$ fleas:

$$
P = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}
\begin{array}{c}
\begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 & 5 \end{array} \\
\begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
1/5 & 0 & 4/5 & 0 & 0 & 0 \\
0 & 2/5 & 0 & 3/5 & 0 & 0 \\
0 & 0 & 3/5 & 0 & 2/5 & 0 \\
0 & 0 & 0 & 4/5 & 0 & 1/5 \\
0 & 0 & 0 & 0 & 1 & 0
\end{pmatrix}
\end{array}.
$$

To find the stationary distribution for the general Ehrenfest chain, let $\boldsymbol{x} = (x_0, x_1, \ldots, x_N)$, with $x_0 = 1$. Set

$$
x_j = \sum_{i=0}^{N} x_i P_{ij} = x_{j-1} \frac{N - (j-1)}{N} + x_{j+1} \frac{j+1}{N}, \tag{3.3}
$$

for $j = 1, \ldots, N-1$. Also, $1 = (1/N)x_1$, so $x_1 = N$. Solving Equation (3.3) starting at $j = 1$ gives $x_2 = N(N-1)/2$, then $x_3 = N(N-1)(N-2)/6$. The general term is

$$
x_j = \frac{N(N-1)\cdots(N-j+1)}{j!} = \frac{N!}{j!(N-j)!} = \binom{N}{j}, \text{ for } j = 0, 1, \ldots, N,
$$

which can be derived by induction. The stationary distribution is

$$
\pi_j = \frac{1}{\sum_{i=0}^{N} \binom{N}{i}} \binom{N}{j} = \binom{N}{j} \frac{1}{2^N}, \text{ for } j = 0, \ldots, N.
$$

The distribution is a binomial distribution with parameters N and 1/2.

The Ehrenfest transition matrix is not regular, and the chain does not have a limiting distribution. However, we can interpret the stationary distribution as giving the long-term proportion of time spent in each state. See Example 3.19 for the description of a modified Ehrenfest scheme, which has a limiting distribution. ■

For the next example, rather than solve a linear system to find the stationary distribution, we take a *guess* at the distribution $\boldsymbol{\pi}$ based on our intuition for how the Markov chain evolves. The candidate distribution $\boldsymbol{\pi}$ is then checked to see if it satisfies $\boldsymbol{\pi} = \boldsymbol{\pi} \boldsymbol{P}$.

> Guessing before proving! Need I remind you that it is so that all important discoveries have been made?
>
> —Henri Poincaré

Example 3.8 (Random walk on a graph) To find the stationary distribution for simple random walk on a graph, consider the interpretation of the distribution as the long-term fraction of time that the walk visits each vertex.

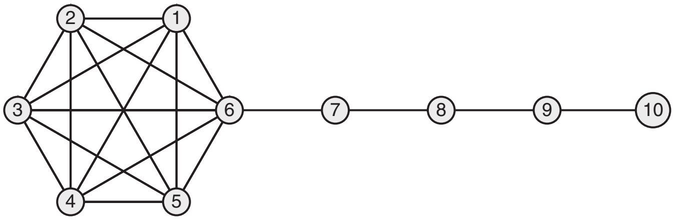

Figure 3.1 Lollipop graph.

For a concrete example, consider the *lollipop graph*, shown in Figure 3.1. One expects that in the long term a random walk on the graph is most likely to be on the *candy* at the leftmost end of the graph, and least likely to be at the right end of the stick. (The candy is a complete graph where all pairs of vertices are joined by edges.)

Intuition suggests that vertices that have more connections are more likely to be visited. That is, the time spent at vertex v is related to the degree of v.

This suggests considering a distribution on vertices that is related to the degree of the vertices. One possibility is a distribution that is proportional to the degree of the vertex. Let

$$\pi_v = \frac{\deg(v)}{\sum_w \deg(w)} = \frac{\deg(v)}{2e},$$

where e is the number of edges in the graph. The sum of the vertex degrees is equal to twice the number of edges since every edge contributes two vertices (its endpoints) to the sum of the vertex degrees.

It remains to check, for this choice of $\boldsymbol{\pi}$, whether in fact $\boldsymbol{\pi} = \boldsymbol{\pi P}$. For vertex v,

$$\begin{aligned}(\pi P)_v &= \sum_w \pi_w P_{wv} = \sum_{w \sim v} \left(\frac{\deg(w)}{2e}\right) \frac{1}{\deg(w)} \\ &= \frac{1}{2e} \sum_{w \sim v} 1 = \frac{\deg(v)}{2e} = \pi_v.\end{aligned}$$

Indeed, our candidate $\boldsymbol{\pi}$ is a stationary distribution.

For the lollipop graph in Figure 3.1, the sum of the vertex degrees is 38. Here is the stationary distribution.

Vertex	1	2	3	4	5	6	7	8	9	10
π_v	5/38	5/38	5/38	5/38	5/38	6/38	2/38	2/38	2/38	1/38

■

Simple random walk on a graph is a special case of random walk on a weighted graph, with edge weights all equal to 1. The stationary distribution for a weighted graph has a similar form as for an unweighted graph. If v is a vertex, say that an edge is *incident* to v if v is an endpoint of the edge.

Stationary Distribution for Random Walk on a Weighted Graph

Let G be a weighted graph with edge weight function $w(i,j)$. For random walk on G, the stationary distribution $\boldsymbol{\pi}$ is proportional to the sum of the edge weights incident to each vertex. That is,

$$\pi_v = \frac{w(v)}{\sum_z w(z)}, \quad \text{for all vertices } v, \tag{3.4}$$

where

$$w(v) = \sum_{z \sim v} w(v, z)$$

is the sum of the edge weights on all edges incident to v.

Stationary Distribution for Simple Random Walk on a Graph

For simple random walk on a nonweighted graph, set $w(i,j) = 1$, for all i, j. Then, $w(v) = \deg(v)$, which gives

$$\pi_v = \frac{\deg(v)}{\sum_z \deg(z)} = \frac{\deg(v)}{2e},$$

where e is the number of edges in the graph.

Example 3.9 The two-state Markov chain with transition matrix

$$\boldsymbol{P} = \begin{array}{c c} & \begin{array}{cc} 1 & 2 \end{array} \\ \begin{array}{c} 1 \\ 2 \end{array} & \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix} \end{array}$$

can be expressed as a random walk on the weighted graph in Figure 3.2. Then, $w(1) = q(1-p) + pq = q$ and $w(2) = pq + p(1-q) = p$. By Equation (3.4), the stationary distribution is

$$\boldsymbol{\pi} = \left(\frac{q}{p+q}, \frac{p}{p+q} \right).$$

■

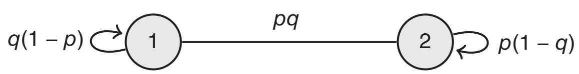

Figure 3.2 The general two-state Markov chain expressed as a weighted graph.

The reader may wonder how the weighted graph in Figure 3.2 is derived from the transition matrix $\boldsymbol{P}$. The algorithm will be explained in Section 3.7.

Example 3.10 Find the stationary distribution for random walk on the hypercube.

Solution The k-hypercube graph, as described in Example 2.8, has 2^k vertices. Each vertex has degree k. The sum of the vertex degrees is $k2^k$, and the stationary distribution $\boldsymbol{\pi}$ is given by

$$\pi_v = \frac{k}{k2^k} = \frac{1}{2^k}, \text{ for all } v.$$

That is, the stationary distribution is uniform on the set of vertices. ∎

The hypercube is an example of a *regular* graph. A graph is regular if all the vertex degrees are the same. For simple random walk on a regular graph, the stationary distribution $\boldsymbol{\pi}$ is uniform on the set of vertices, since π_j is constant for all j. In addition to the hypercube, examples of regular graphs with uniform stationary distributions include the cycle graph ($\deg(v) = 2$) and the complete graph on k vertices ($\deg(v) = k - 1$).

The Eigenvalue Connection*

The stationary distribution of a Markov chain is related to the eigenstructure of the transition matrix.

First, a reminder on notation. For a matrix $\boldsymbol{M}$, the *transpose* of $\boldsymbol{M}$ is denoted $\boldsymbol{M}^T$. In this book, vectors are considered as row vectors. If $\boldsymbol{x}$ is a vector, $\boldsymbol{x}^T$ is a column vector.

Recall that an eigenvector of $\boldsymbol{M}$ is a column vector $\boldsymbol{x}^T$ such that $\boldsymbol{M}\boldsymbol{x}^T = \lambda \boldsymbol{x}^T$, for some scalar λ. We call such a vector a *right eigenvector* of $\boldsymbol{M}$. A *left eigenvector* of $\boldsymbol{M}$ is a row vector $\boldsymbol{y}$, which satisfies $\boldsymbol{y}\boldsymbol{M} = \mu \boldsymbol{y}$, for some scalar μ. A left eigenvector of $\boldsymbol{M}$ is simply a right eigenvector of $\boldsymbol{M}^T$.

If $\boldsymbol{\pi}$ is the stationary distribution of a Markov chain and satisfies $\boldsymbol{\pi}\boldsymbol{P} = \boldsymbol{\pi}$, then $\boldsymbol{\pi}$ is a left eigenvector of $\boldsymbol{P}$ corresponding to eigenvalue $\lambda = 1$.

Let $\mathbf{1}$ denote the column vector of all 1s. Since the rows of a stochastic matrix sum to 1, $\boldsymbol{P}\mathbf{1} = \mathbf{1} = (1)\mathbf{1}$. That is, $\mathbf{1}$ is a right eigenvector of $\boldsymbol{P}$ corresponding to eigenvalue $\lambda = 1$.

A matrix and its transpose have the same set of eigenvalues, with possibly different eigenvectors. It follows that $\lambda = 1$ is an eigenvalue of $\boldsymbol{P}^T$ with some corresponding right eigenvector $\boldsymbol{y}^T$. Equivalently, $\boldsymbol{y}$ is a left eigenvector of $\boldsymbol{P}$. That is, there exists a row vector $\boldsymbol{y}$ such that $\boldsymbol{y}\boldsymbol{P} = \boldsymbol{y}$. If a multiple of $\boldsymbol{y}$ can be normalized so that its components are non-negative and sum to 1, then this gives a stationary distribution. However, some of the entries of $\boldsymbol{y}$ might be negative, or complex-valued, and the vector might not be able to be normalized to give a probability distribution.

If a Markov chain has a unique stationary distribution, then the distribution is an eigenvector of $\boldsymbol{P}^T$ corresponding to $\lambda = 1$.

R: Stationary Distribution and Eigenvectors

The R command `eigen(P)` returns the eigenvalues and eigenvectors of a square matrix P. These are given in a list with two components: `values` contains the eigenvalues, and `vectors` contains the corresponding eigenvectors stored as a matrix. If P is a stochastic matrix, an eigenvector corresponding to eigenvalue $\lambda = 1$ will be stored in the first column of the `vectors` matrix. The R command `t(P)` gives the transpose of P.

In the following, an eigenvector is found for $\boldsymbol{P}^T$ corresponding to $\lambda = 1$. The vector is then normalized so that components sum to 1 in order to compute the stationary distribution. We illustrate on the weather matrix with stationary distribution $\boldsymbol{\pi} = (1/9, 3/4, 5/36) = (0.111,\ 0.750,\ 0.139)$.

```
> P
      Rain Snow Clear
Rain   0.2  0.6   0.2
Snow   0.1  0.8   0.1
Clear  0.1  0.6   0.3
> eigen(P)
$values
[1] 1.0 0.2 0.1
$vectors
          [,1]       [,2]       [,3]
[1,] 0.5773503  0.6882472 -0.9847319
[2,] 0.5773503 -0.2294157  0.1230915
[3,] 0.5773503  0.6882472  0.1230915
> eigen(P)$values  # eigenvalues
[1] 1.0 0.2 0.1
# eigenvalues of P and its transpose are the same
> eigen(t(P))$values
[1] 1.0 0.2 0.1
# eigenvectors of P-transpose
> eigen(t(P))$vectors
          [,1]          [,2]          [,3]
[1,] 0.1441500 -2.008469e-16  7.071068e-01
[2,] 0.9730125 -7.071068e-01  3.604182e-16
[3,] 0.1801875  7.071068e-01 -7.071068e-01

# first column gives eigenvector for eigenvalue 1
> x <- eigen(t(P))$vectors[,1]
> x
[1] 0.1441500 0.9730125 0.1801875
# normalize so rows sum to 1
> x/sum(x)
```

```
[1] 0.1111111 0.7500000 0.1388889

#  one-line command to find stationary distribution
> x <- eigen(t(P))$vectors[,1]; x/sum(x)
[1] 0.1111111 0.7500000 0.1388889
```

3.3 CAN YOU FIND THE WAY TO STATE *a*?

The long-term behavior of a Markov chain is related to how often states are visited. Here, we look more closely at the relationship between states and how reachable, or accessible, groups of states are from each other.

Say that state j is *accessible* from state i, if $P_{ij}^n > 0$, for some $n \geq 0$. That is, there is positive probability of reaching j from i in a finite number of steps. States i and j *communicate* if i is accessible from j and j is accessible from i.

Communication is an equivalence relation, which means that it satisfies the following three properties.

1. *(Reflexive)* Every state communicates with itself.
2. *(Symmetric)* If i communicates with j, then j communicates with i.
3. *(Transitive)* If i communicates with j, and j communicates with k, then i communicates with k.

Property 1 holds since $P_{ii}^0 = P(X_0 = i|X_0 = i) = 1$. Property 2 follows since the definition of communication is symmetric. For Property 3, assume that i communicates with j, and j communicates with k. Then, there exists $n \geq 0$ and $m \geq 0$ such that $P_{ij}^n > 0$ and $P_{jk}^m > 0$. Therefore,

$$P_{ik}^{n+m} = \sum_t P_{it}^n P_{tk}^m \geq P_{ij}^n P_{jk}^m > 0.$$

Thus, k is accessible from i. Similarly, i is accessible from k.

Since communication is an equivalence relation the state space can be partitioned into equivalence classes, called *communication classes*. That is, the state space can be divided into disjoint subsets, each of whose states communicate with each other but do not communicate with any states outside their class.

A modified transition graph is a useful tool for finding the communication classes of a Markov chain. Vertices of the graph are the states of the chain. A directed edge is drawn between i and j if $P_{ij} > 0$. For purposes of studying the communication relationship between states, it is not necessary to label the edges with probabilities.

Example 3.11 Find the communication classes for the Markov chains with these transition matrices.

$$
P = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \end{array}
\begin{array}{c} \begin{array}{ccccc} a & b & c & d & e \end{array} \\
\begin{pmatrix} 0 & 0 & 0 & 2/3 & 1/3 \\ 1/2 & 0 & 1/6 & 0 & 1/3 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 3/4 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array},
\quad
Q = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \\ f \end{array}
\begin{array}{c} \begin{array}{cccccc} a & b & c & d & e & f \end{array} \\
\begin{pmatrix} 1/6 & 1/3 & 0 & 0 & 1/2 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3/4 & 1/4 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 4/5 & 0 & 0 & 1/5 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 & 0 \end{pmatrix} \end{array}.
$$

Solution The transition graphs are shown in Figure 3.3. For the $\boldsymbol{P}$-chain, the communication classes are $\{a, b, c, d\}$ and $\{e\}$. For the $\boldsymbol{Q}$-chain, the communication classes are $\{a, d, e\}$, $\{b\}$, and $\{c, f\}$.

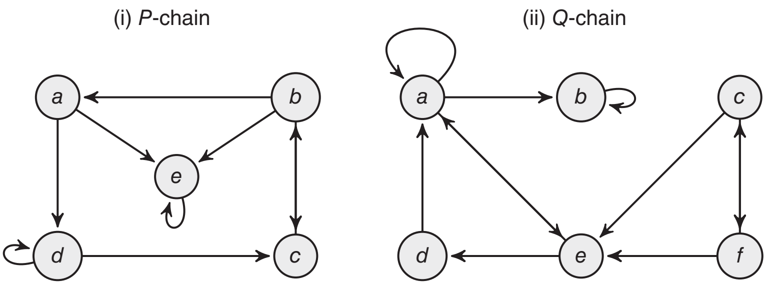

Figure 3.3 Transition graphs.

■

Most important is the case when the states of a Markov chain all communicate with each other.

Irreducibility

A Markov chain is called *irreducible* if it has exactly one communication class. That is, all states communicate with each other.

Example 3.12 The Markov chain with transition matrix

$$
P = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \\ f \end{array}
\begin{array}{c} \begin{array}{cccccc} a & b & c & d & e & f \end{array} \\
\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1/4 & 1/4 & 0 & 1/4 & 0 & 1/4 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \end{array}
$$

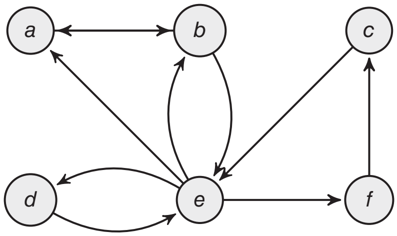

Figure 3.4 Transition graph for an irreducible Markov chain.

is irreducible, which can be seen by examining the transition graph in Figure 3.4.

■

Recurrence and Transience

Consider the transition graph in Figure 3.5. The communication classes are $\{a, b\}$ and $\{c\}$. From each state, consider the evolution of the chain started from that state and the probability that the chain eventually revisits that state.

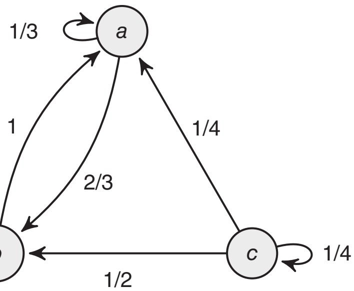

Figure 3.5

From a, the chain either returns to a in one step, or first moves to b and then returns to a on the second step. From a, the chain revisits a, with probability 1.

For the chain started in b, the chain first moves to a. It may continue to revisit a for many steps, but eventually it will return to b. This is because the probability that the chain stays at a forever is the probability that it continually transitions from a to a, which is equal to

$$\lim_{n\to\infty} (P_{aa})^n = \lim_{n\to\infty} \left(\frac{1}{3}\right)^n = 0.$$

Thus, from b, the chain revisits b, with probability 1.

For the chain started in c, the chain may revisit c for many successive steps. But with positive probability it will eventually move to either a or b. Once it does, it will never revisit c, as it is now *stuck* in the $\{a, b\}$ communication class. From c, there is positive probability that the chain started in c will never revisit c. In this case, that probability is $1 - 1/4 = 3/4$.

The states of a Markov chain, as this example illustrates, exhibit one of two contrasting behaviors. For the chain started in a given state, the chain either revisits that state, with probability 1, or there is positive probability that the chain will never revisit that state.

Given a Markov chain $X_0, X_1, \ldots$, let $T_j = \min\{n > 0 : X_n = j\}$ be the *first passage time* to state j. If $X_n \neq j$, for all $n > 0$, set $T_j = \infty$. Let

$$f_j = P(T_j < \infty | X_0 = j)$$

be the probability that the chain started in j eventually returns to j. For the three-state chain introduced in this section, $f_a = f_b = 1$, and $f_c = 1/4$. We classify the states j of a Markov chain according to whether or not $f_j = 1$.

Recurrent and Transient States

State j is said to be *recurrent* if the Markov chain started in j eventually revisits j. That is, $f_j = 1$.

State j is said to be *transient* if there is positive probability that the Markov chain started in j never returns to j. That is, $f_j < 1$.

Whether or not a state is eventually revisited is strongly related to how often that state is visited.

For the chain started in i, let

$$I_n = \begin{cases} 1, & \text{if} \quad X_n = j, \\ 0, & \text{otherwise,} \end{cases}$$

for $n \geq 0$. Then, $\sum_{n=0}^{\infty} I_n$ is the number of visits to j. The expected number of visits to j is

$$E\left(\sum_{n=0}^{\infty} I_n\right) = \sum_{n=0}^{\infty} E(I_n) = \sum_{n=0}^{\infty} P(X_n = j | X_0 = i) = \sum_{n=0}^{\infty} P_{ij}^n,$$

where the infinite sum may possibly diverge to $+\infty$. For the chain started in i, the expected number of visits to j is the ijth entry of the matrix $\sum_{n=0}^{\infty} \boldsymbol{P}^n$.

Assume that j is recurrent. The chain started at j will eventually revisit j with probability 1. Once it hits j, the chain begins anew and behaves as if a new version of the chain started at j. We say the Markov chain *regenerates* itself. (This intuitive behavior is known as the *strong Markov property*. For a more formal treatment see Section 3.9.) From j, the chain will revisit j again, with probability 1, and so on. It follows that j will be visited infinitely many times, and

$$\sum_{n=0}^{\infty} P_{jj}^n = \infty.$$

On the other hand, assume that j is transient. Starting at j, the probability of eventually hitting j again is f_j, and the probability of never hitting j is $1 - f_j$. If the chain hits j, the event that it will eventually revisit j is independent of past history. It follows that the sequence of successive visits to j behaves like an i.i.d. sequence of coin tosses where heads occurs if j is eventually hit and tails occurs if j is never hit again. The number of times that j is hit is the number of coin tosses until tails occurs, which has a geometric distribution with parameter $1 - f_j$. Thus, the expected number of visits to j is $1/(1 - f_j)$, and

$$\sum_{n=0}^{\infty} P_{jj}^n = \frac{1}{1 - f_j} < \infty.$$

In particular, a transient state will only be visited a finite number of times.

This leads to another characterization of recurrence and transience.

Recurrence, Transience

(i) State j is recurrent if and only if

$$\sum_{n=0}^{\infty} P_{jj}^n = \infty.$$

(ii) State j is transient if and only if

$$\sum_{n=0}^{\infty} P_{jj}^n < \infty.$$

Assume that j is recurrent and accessible from i. For the chain started in i there is positive probability of hitting j. And from j, the expected number of visits to j is infinite. It follows that the expected number of visits to j for the chain started in i is also infinite, and thus

$$\sum_{n=0}^{\infty} P_{ij}^n = \infty.$$

Assume that j is transient and accessible from i. By a similar argument the expected number of visits to j for the chain started in i is finite, and thus

$$\sum_{n=0}^{\infty} P_{ij}^n < \infty,$$

from which it follows that

$$\lim_{n \to \infty} P_{ij}^n = 0. \tag{3.5}$$

The long-term probability that a Markov chain eventually hits a transient state is 0.

Recurrence and transience are *class* properties of a Markov chain as described by the following theorem.

Recurrence and Transience are Class Properties

Theorem 3.3. *The states of a communication class are either all recurrent or all transient.*

Proof. Let i and j be states in the same communication class. Assume that i is recurrent. Since i and j communicate, there exists $r \geq 0$ and $s \geq 0$ such that $P^r_{ji} > 0$ and $P^s_{ij} > 0$. For $n \geq 0$,

$$P^{r+n+s}_{jj} = \sum_k \sum_l P^r_{jk} P^n_{kl} P^s_{lj} \geq P^r_{ji} P^n_{ii} P^s_{ij}.$$

Summing over n gives

$$\sum_{n=0}^{\infty} P^{r+n+s}_{jj} \geq P^r_{ji} \left(\sum_{n=0}^{\infty} P^n_{ii} \right) P^s_{ji} = \infty.$$

Since

$$\sum_{n=0}^{\infty} P^n_{jj} \geq \sum_{n=r+s}^{\infty} P^n_{jj} = \sum_{n=0}^{\infty} P^{r+n+s}_{jj},$$

it follows that $\sum_{n=0}^{\infty} P^n_{jj}$ diverges to infinity, and thus j is recurrent. Hence, if one state of a communication class is recurrent, all states in that class are recurrent.

On the other hand, if one state is transient, the other states must be transient. By contradiction, if the communication class contains a recurrent state then by what was just proven all the states are recurrent. ■

Corollary 3.4. *For a finite irreducible Markov chain, all states are recurrent.*

Proof. The states of an irreducible chain are either all recurrent or all transient. Assume that they are all transient. Then, state 1 will be visited for a finite amount of time, after which it is never hit again, similarly with state 2, and with all states. Since there are finitely many states, it follows that *none* of the states will be visited after some finite amount of time, which is not possible. ■

By Corollary 3.4, a finite Markov chain cannot have all transient states. This is not true for infinite chains, as the following classic example illustrates.

Example 3.13 (Simple random walk) A random walk on the integer line starts at 0 and moves left, with probability p, or right, with probability $1 - p$. For $0 < p < 1$, the process is an irreducible Markov chain, as every state is accessible from every other state. Is the chain recurrent or transient?

Solution Since the chain is irreducible, it suffices to examine one state. Choose state 0 and consider $\sum_{n=0}^{\infty} P_{00}^{n}$. Observe that from 0 the walk can only revisit 0 in an even number of steps. So $P_{00}^{n} = 0$, if n is odd. To move from 0 to 0 in exactly $2n$ steps requires that the walk moves n steps to the left and n steps to the right, in some order. Such a path of length $2n$ can be identified with a sequence of n Ls and n Rs. There are $\binom{2n}{n}$ such sequences. Each left move occurs with probability p and each right move occurs with probability $1 - p$. This gives

$$P_{00}^{2n} = \binom{2n}{n} p^n (1-p)^n.$$

The binomial coefficient $\binom{2n}{n}$ is estimated using *Stirling's approximation*

$$n! \approx n^n e^{-n} \sqrt{2\pi n}, \text{ for large } n.$$

The more precise statement is

$$\lim_{n\to\infty} \frac{n!}{n^n e^{-n} \sqrt{2\pi n}} = 1.$$

By Stirling's approximation, for large n,

$$\binom{2n}{n} = \frac{(2n)!}{n!n!} \approx \frac{(2n)^{2n} e^{-2n} \sqrt{2\pi 2n}}{\left(n^n e^{-n} \sqrt{2\pi n}\right)^2} = \frac{4^n}{\sqrt{\pi n}}.$$

Thus,

$$\sum_{n=0}^{\infty} P_{00}^{2n} = \sum_{n=0}^{\infty} \binom{2n}{n} p^n (1-p)^n \approx \sum_{n=1}^{\infty} \frac{(4p(1-p))^n}{\sqrt{\pi n}}.$$

Convergence of the infinite series depends upon p. We have

$$\sum_{n=0}^{\infty} P_{00}^{2n} \approx \begin{cases} \sum_{n=1}^{\infty} \frac{1}{\sqrt{\pi n}} = \infty, & \text{if } p = 1/2, \\ \sum_{n=1}^{\infty} \frac{\epsilon^n}{\sqrt{\pi n}} < \infty, & \text{if } p \neq 1/2, \end{cases}$$

where $\epsilon = 4p(1-p)$. If $p \neq 1/2$, then $0 < \epsilon < 1$, and $\epsilon^n \to 0$, as $n \to \infty$.

For $p = 1/2$, the random walk is recurrent. Each integer, no matter how large, is visited infinitely often. For $p \neq 1/2$, the walk is transient. With positive probability the walk will never return to its starting point.

Surprises await for random walk in higher dimensions. Simple symmetric random walk on the integer points in the plane $\mathbb{Z}^2$ moves left, right, up, or down, with probability 1/4 each. The process has been called the *drunkard's walk*. As in one dimension, the walk is recurrent. The method of proof is similar. See Exercise 3.20. Letting 0 denote the origin in the plane, it can be shown that

$$\sum_{n=0}^{\infty} P_{00}^{n} \approx \sum_{n=1}^{\infty} \frac{1}{\pi n} = \infty.$$

Remarkably, in dimensions three and higher simple symmetric random walk is transient. This was first shown by George Pólya in 1921 and is known as *Pólya's Theorem*. It can be shown that in $\mathbb{Z}^3$,

$$\sum_{n=0}^{\infty} P_{00}^{n} \approx \sum_{n=1}^{\infty} \frac{1}{(\pi n)^{3/2}} < \infty.$$

The mathematician Shizuo Kakutani is quoted as explaining this result by saying, "A drunk man will find his way home, but a drunk bird may get lost forever." ■

Canonical Decomposition

A set of states C is said to be *closed* if no state outside of C is accessible from any state in C. If C is closed, then $P_{ij} = 0$ for all $i \in C$ and $j \notin C$.

Closed Communication Class

Lemma 3.5. *A communication class is closed if it consists of all recurrent states. A finite communication class is closed only if it consist of all recurrent states.*

Proof. Let C be a communication class made up of recurrent states. Assume that C is not closed. Then, there exists states $i \in C$ and $j \notin C$ such that $P_{ij} > 0$. Since j is accessible from i, i is not accessible from j, otherwise j would be contained in C. Start the chain in i. With positive probability, the chain will hit j and then never hit i again. But this contradicts the assumption that i is recurrent.

On the other hand, assume that C is closed and finite. By the same argument given in the proof of Corollary 3.4 the states cannot all be transient. Hence, they are all recurrent. ■

The state space $\mathcal{S}$ of a finite Markov chain can be partitioned into transient and recurrent states as $\mathcal{S} = T \cup R_1 \cup \cdots \cup R_m$, where T is the set of all transient states and the R_i are closed communication classes of recurrent states. This is called the *canonical decomposition*. The computation of many quantities associated with Markov chains can be simplified by this decomposition.

Given a canonical decomposition, the state space can be reordered so that the Markov transition matrix has the block matrix form

$$\boldsymbol{P} = \begin{array}{c} \\ T \\ R_1 \\ \vdots \\ R_m \end{array} \begin{array}{c} \begin{array}{cccc} T & R_1 & \cdots & R_m \end{array} \\ \begin{pmatrix} * & * & \cdots & * \\ \mathbf{0} & \boldsymbol{P}_1 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{P}_m \end{pmatrix} \end{array}.$$

Each submatrix $\boldsymbol{P}_1, \dots, \boldsymbol{P}_m$ is a square stochastic matrix corresponding to a closed recurrent communication class. By itself, each of these matrices is the matrix of an irreducible Markov chain with a restricted state space.

Example 3.14 Consider the Markov chain with transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \\ f \\ g \end{array} \begin{array}{c} \begin{array}{ccccccc} a & b & c & d & e & f & g \end{array} \\ \begin{pmatrix} 1/4 & 0 & 0 & 0 & 0 & 0 & 3/4 \\ 1/8 & 1/8 & 1/4 & 0 & 1/4 & 1/8 & 1/8 \\ 0 & 0 & 2/5 & 1/5 & 2/5 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 & 0 \\ 0 & 1/5 & 0 & 1/5 & 1/5 & 1/5 & 1/5 \\ 4/5 & 0 & 0 & 0 & 0 & 0 & 1/5 \end{pmatrix} \end{array}$$

described by the transition graph in Figure 3.6. Give the canonical decomposition.

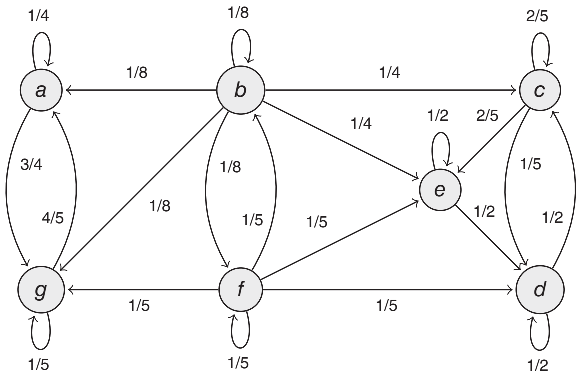

Figure 3.6

Solution States b and f are transient. The closed recurrent classes are $\{a, g\}$ and $\{c, d, e\}$. Reordering states gives the transition matrix in block matrix form

$$\boldsymbol{P} = \begin{array}{c} \\ b \\ f \\ a \\ g \\ c \\ d \\ e \end{array} \begin{array}{c} \begin{array}{ccccccc} b & f & a & g & c & d & e \end{array} \\ \begin{pmatrix} 1/8 & 1/8 & 1/8 & 1/8 & 1/4 & 0 & 1/4 \\ 1/5 & 1/5 & 0 & 1/5 & 0 & 1/5 & 1/5 \\ 0 & 0 & 1/4 & 3/4 & 0 & 0 & 0 \\ 0 & 0 & 4/5 & 1/5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2/5 & 1/5 & 2/5 \\ 0 & 0 & 0 & 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 \end{pmatrix} \end{array}.$$

■

The canonical decomposition is useful for describing the long-term behavior of a Markov chain. The block matrix form facilitates taking matrix powers. For $n \geq 1$,

$$\boldsymbol{P}^n = \begin{array}{c} \\ T \\ R_1 \\ \vdots \\ R_m \end{array} \begin{array}{c} \begin{array}{cccc} T & R_1 & \cdots & R_m \end{array} \\ \begin{pmatrix} * & * & \cdots & * \\ \mathbf{0} & \boldsymbol{P}_1^n & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{P}_m^n \end{pmatrix} \end{array}.$$

Taking limits gives

$$\lim_{n\to\infty} \boldsymbol{P}^n = \begin{array}{c} \\ T \\ R_1 \\ \vdots \\ R_m \end{array} \begin{array}{c} \begin{array}{cccc} T & R_1 & \cdots & R_m \end{array} \\ \begin{pmatrix} \mathbf{0} & * & \cdots & * \\ \mathbf{0} & \lim_{n\to\infty} \boldsymbol{P}_1^n & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \lim_{n\to\infty} \boldsymbol{P}_m^n \end{pmatrix} \end{array}.$$

Note that the entries of the columns corresponding to transient states are all 0 as a consequence of Equation (3.5).

The recurrent, closed communication classes $R_1, \ldots, R_m$ behave like mini-irreducible Markov chains where all states communicate with each other. The asymptotic properties of the submatrices $\boldsymbol{P}_1, \ldots, \boldsymbol{P}_m$ lead us to consider the properties of irreducible Markov chains, which is where our path now goes.

3.4 IRREDUCIBLE MARKOV CHAINS

The next theorem characterizes the stationary distribution $\boldsymbol{\pi}$ for finite irreducible Markov chains. It relates the stationary probability π_j to the expected number of steps between visits to j. Recall that $T_j = \min\{n > 0 : X_n = j\}$ is the first passage time to state j.

Limit Theorem for Finite Irreducible Markov Chains

Theorem 3.6. *Assume that $X_0, X_1, \ldots$ is a finite irreducible Markov chain. For each state j, let $\mu_j = E(T_j|X_0 = j)$ be the expected return time to j. Then, μ_j is finite, and there exists a unique, positive stationary distribution $\boldsymbol{\pi}$ such that*

$$\pi_j = \frac{1}{\mu_j}, \quad \textit{for all } j. \tag{3.6}$$

Furthermore, for all states i,

$$\pi_j = \lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} P_{ij}^m. \tag{3.7}$$

The theorem is proved in Section 3.10.

Remark:

1. The fact that $\pi_j = 1/\mu_j$ is intuitive. If there is one visit to j every μ_j steps, then the proportion of visits to j is $1/\mu_j$.
2. The theorem does not assert that $\boldsymbol{\pi}$ is a limiting distribution. The convergence in Equation (3.7) is a weaker form of convergence than $\pi_j = \lim_{n\to\infty} P^n_{ij}$. We discuss in the next section that an additional assumption is needed for $\boldsymbol{\pi}$ to be a limiting distribution.
3. For finite irreducible Markov chains, all states are recurrent, and the expected return time $E(T_j|X_0 = j)$ is finite, for all j. However, for an infinite Markov chain if j is a recurrent state, even though the chain will eventually revisit j with probability 1, the expected number of steps between such visits need not be finite. The theorem can be extended to infinite irreducible Markov chains for which the expected return time $E(T_j|X_0 = j)$ is finite, for all j.

   A recurrent state j is called *positive recurrent* if $E(T_j|X_0 = j) < \infty$, and *null recurrent* if $E(T_j|X_0 = j) = \infty$. Thus, the theorem holds for irreducible Markov chains for which all states are positive recurrent. See Exercise 3.27 for an example of a Markov chain in which all states are null recurrent.

In many applications, the expected time between visits to a given state is of particular importance.

Example 3.15 (Earthquake recurrences) The Chiayi–Tainan area of Taiwan was devastated by an earthquake on September 21, 1999. In Tsai (2002), Markov chains were used to study seismic activity in the region. A chain is constructed with states corresponding to Richter scale magnitudes of earthquake intensity. The state space is $\{M_2, M_3, M_4, M_5\}$, where M_k denotes an earthquake with a Richter level in the interval $[k, k + 1)$. A Markov transition matrix is estimated from historical data for the period 1973–1975:

$$\boldsymbol{P} = \begin{array}{c} \\ M_2 \\ M_3 \\ M_4 \\ M_5 \end{array}\!\!\begin{array}{c} \begin{array}{cccc} M_2 & M_3 & M_4 & M_5 \end{array} \\ \begin{pmatrix} 0.785 & 0.194 & 0.018 & 0.003 \\ 0.615 & 0.334 & 0.048 & 0.003 \\ 0.578 & 0.353 & 0.069 & 0.000 \\ 0.909 & 0.000 & 0.091 & 0.000 \end{pmatrix} \end{array}.$$

The stationary distribution $\boldsymbol{\pi} = (0.740, 0.230, 0.027, 0.003)$ is found with technology. Earthquakes of magnitude M_2 or greater tend to occur in this region about once every four months. If an M_5 earthquake occurs, investigators would like to know how long it will be before another M_5 earthquake.

The expected number of Markov chain transitions between M_5 earthquakes is $1/\pi_{M_5} = 1/0.003 = 333$. If earthquakes occur, on average, every four months, then according to the model it will take about $333 \times (4/12) = 111$ years before another M_5 earthquake. ■

Example 3.16 For the frog-jumping random walk on an n-cycle, how many hops does it take, on average, for the frog to return to its starting lily pad?

Solution In the cycle graph, all vertices have the same degree. Hence, for simple random walk on the cycle, the stationary distribution is uniform on the set of vertices. Since $\pi_v = 1/n$, for all vertices v, it takes the frog, on average, $1/\pi_v = n$ hops to return to its starting pad. ■

First-Step Analysis

The expected return time $E(T_j|X_0 = j)$ is found by taking the reciprocal of the stationary probability π_j. Another approach is to condition on the first step of the chain and use the law of total expectation. This is called *first-step analysis*.

Example 3.17 Consider a Markov chain with transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ a \\ b \\ c \end{array} \begin{array}{c} \begin{array}{ccc} a & b & c \end{array} \\ \begin{pmatrix} 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \\ 1/3 & 1/3 & 1/3 \end{pmatrix} \end{array}.$$

From state a, find the expected return time $E(T_a|X_0 = a)$ using first-step analysis.

Solution Let $e_x = E(T_a|X_0 = x)$, for $x = a, b, c$. Thus, e_a is the desired expected return time, and e_b and e_c are the expected *first passage* times to a for the chain started in b and c, respectively.

For the chain started in a, the next state is b, with probability 1. From b, the further evolution of the chain behaves as if the original chain started at b. Thus,

$$e_a = 1 + e_b.$$

From b, the chain either hits a, with probability $1/2$, or moves to c, where the chain behaves as if the original chain started at c. It follows that

$$e_b = \frac{1}{2} + \frac{1}{2}(1 + e_c).$$

Similarly, from c, we have

$$e_c = \frac{1}{3} + \frac{1}{3}(1 + e_b) + \frac{1}{3}(1 + e_c).$$

Solving the three equations gives

$$e_c = \frac{8}{3}, \quad e_b = \frac{7}{3}, \quad \text{and} \quad e_a = \frac{10}{3}.$$

The desired expected return time is $10/3$.

We leave it to the reader to verify that the stationary distribution is

$$\pi = \left(\frac{3}{10}, \frac{2}{5}, \frac{3}{10}\right).$$

The expected return time is simulated in the following `R` code. The chain started at a is run for 25 steps (long enough to return to a with very high probability), and the return time to a is found. The mean return time is estimated based on 10,000 trials.

R : Simulating an Expected Return Time

```
#returntime.R
> P
        a       b       c
a 0.00000 1.00000 0.00000
b 0.50000 0.00000 0.50000
c 0.33333 0.33333 0.33333
> init
[1] 1 0 0
> states
[1] "a" "b" "c"
> markov(init,P,25,states)
 "a" "b" "c" "c" "c" "b" "a" "b" "a" "b" "a" "b" "c"
 "b" "c" "a" "b" "c" "b" "c" "b" "a" "b" "a" "b" "a"

> trials <- 10000
> simlist <- numeric(trials)
> for (i in 1:trials) {
   path <- markov(init,P,25,states)
     # find the index of the 2nd occurrence of "a"
     # subtract 1 to account for time 0
   returntime <- which(path == "a")[2] - 1
   simlist[i] <- returntime }
# expected return time to state a
> mean(simlist)
[1] 3.3346
```

■

3.5 PERIODICITY

Finite irreducible Markov chains have unique, positive stationary distributions. Although they may not have limiting distributions, they have almost limiting behavior in the sense that for all states i and j, the partial averages $(1/n)\sum_{m=0}^{n-1} P_{ij}^m$ converge.

An example of a finite irreducible Markov chain with no limiting distribution is random walk on the n-cycle, when n is even. The graph is regular (all vertex degrees are the same) and the unique stationary distribution is uniform. But there is no limiting distribution since the chain flip-flops back and forth between even and odd states. The chain's position after n steps depends on the parity of the initial state.

It is precisely the finite irreducible Markov chains that do not exhibit this type of *periodic* behavior, which have limiting distributions.

For a Markov chain started in state i, consider the set of times when the chain can return to i. For the chain described by the graph in Figure 3.7a, from any state the set of possible return times is $\{2, 4, 6, 8, \dots\}$. The same is true for the chain in Figure 3.7b. The chain started from any state returns to that state in multiples of two steps. For the chain in Figure 3.7c, from each state the set of return times is $\{3, 6, 9, 12, \dots\}$ The chain started in a returns to a in multiples of three steps.

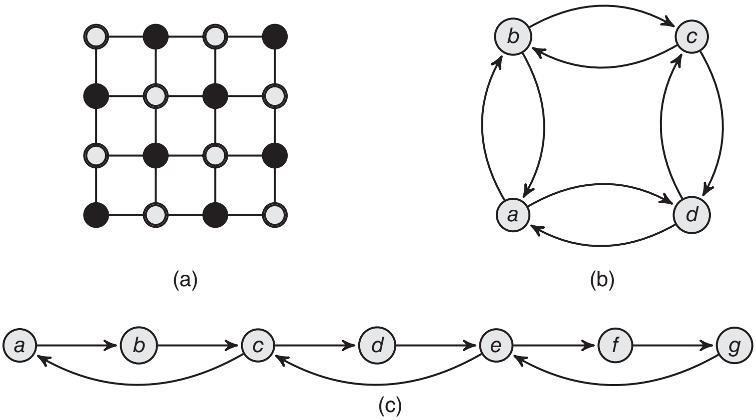

Figure 3.7 Periodic Markov chains.

The idea is formalized in the following definition. Recall that the *greatest common divisor (gcd)* of a set of positive integers is the largest integer that divides all the numbers of the set without a remainder.

Period

For a Markov chain with transition matrix $\boldsymbol{P}$, the *period* of state i, denoted $d(i)$, is the greatest common divisor of the set of possible return times to i. That is,

$$d(i) = \gcd\{n > 0 : P^n_{ii} > 0\}.$$

If $d(i) = 1$, state i is said to be *aperiodic*. If the set of return times is empty, set $d(i) = +\infty$.

The definition of period gives that from state i, returns to i can only occur in multiples of $d(i)$ steps. And the period $d(i)$ is the largest such number with this property.

Periodicity, similar to recurrence and transience, is a class property.

Periodicity is a Class Property

Lemma 3.7. *The states of a communication class all have the same period.*

Proof. Let i and j be states in the same communication class with respective periods $d(i)$ and $d(j)$. Since i and j communicate, there exist positive integers r and s, such that $P^r_{ij} > 0$ and $P^s_{ji} > 0$. Then,

$$P^{r+s}_{ii} = \sum_k P^r_{ik}P^s_{ki} \geq P^r_{ij}P^s_{ji} > 0.$$

Thus $r + s$ is a possible return time for i, and hence $d(i)$ is a divisor of $r + s$. Assume that $P^n_{jj} > 0$ for some positive integer n. Then,

$$P^{r+s+n}_{ii} \geq P^r_{ij}P^n_{jj}P^s_{ji} > 0,$$

and thus $d(i)$ is a divisor of $r + s + n$. Since $d(i)$ divides both $r + s$ and $r + s + n$, it must also divide n. Thus, $d(i)$ is a common divisor of the set $\{n > 0 : P^n_{jj} > 0\}$. Since $d(j)$ is the largest such divisor, it follows that $d(i) \leq d(j)$. By the same argument with i and j reversed, we have that $d(j) \leq d(i)$. Hence, $d(i) = d(j)$. ■

Example 3.18 Consider the transition graph in Figure 3.8. Identify the communication classes, their periods, and whether the class is recurrent or transient.

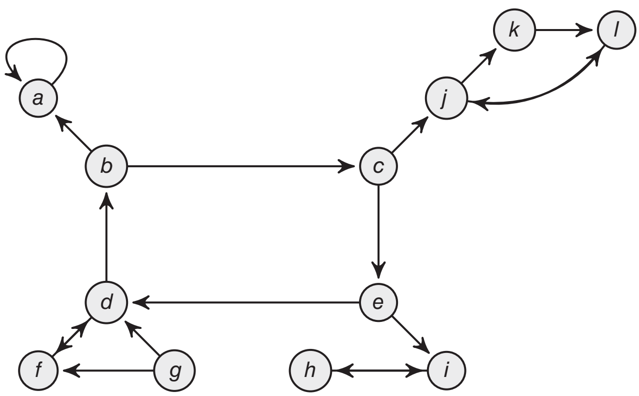

Figure 3.8

Solution Communication classes, with periods, are as follows:

(i) $\{a\}$ is recurrent with period 1,
(ii) $\{b, c, d, e, f\}$ is transient with period 2,

(iii) $\{g\}$ is transient with period $+\infty$,
(iv) $\{h, i\}$ is recurrent with period 2, and
(v) $\{j, k, l\}$ is recurrent with period 1.

Observe that return times for state j can occur in multiples of three (first k, then l, then j) or in multiples of two (first l then j). Since two and three are relatively prime, their great common divisor is one. Hence, $d(j) = d(k) = d(l) = 1$. ■

From Lemma 3.7, it follows that all states in an irreducible Markov chain have the same period.

Periodic, Aperiodic Markov Chain

A Markov chain is called *periodic* if it is irreducible and all states have period greater than 1.

A Markov chain is called *aperiodic* if it is irreducible and all states have period equal to 1.

Note that any state i with the property that $P_{ii} > 0$ is necessarily aperiodic. Thus, a sufficient condition for an irreducible Markov chain to be aperiodic is that $P_{ii} > 0$ for some i. That is, at least one diagonal entry of the transition matrix is nonzero.

3.6 ERGODIC MARKOV CHAINS

A Markov chain is called *ergodic* if it is irreducible, aperiodic, and all states have finite expected return times. The latter is always true for finite chains. Thus, a finite Markov chain is ergodic if it is irreducible and aperiodic. It is precisely the class of ergodic Markov chains that have positive limiting distributions.

Fundamental Limit Theorem for Ergodic Markov Chains

Theorem 3.8. *Let $X_0, X_1, \ldots$ be an ergodic Markov chain. There exists a unique, positive, stationary distribution $\boldsymbol{\pi}$, which is the limiting distribution of the chain. That is,*

$$\pi_j = \lim_{n\to\infty} P^n_{ij}, \text{ for all } i, j.$$

Recall Theorem 3.2, which asserts the same limit result for Markov chains with regular transition matrices. The proof of the fundamental limit theorem for ergodic

Markov chains is given in Section 3.10, where it is also shown that a Markov chain is ergodic if and only if its transition matrix is regular.

Example 3.19 (Modified Ehrenfest model) In the Ehrenfest scheme of Example 3.7, at each discrete step one of N fleas is picked uniformly at random. The flea jumps from one dog to the other. Our dogs are named Cooper and Lisa. Let X_n be the number of fleas on Lisa after n jumps.

The Ehrenfest chain $X_0, X_1, \ldots$ is irreducible and periodic with period 2. From state 0, the chain can only return to 0 in an even number of steps.

A modified Ehrenfest scheme picks a flea uniformly at random and then picks a dog uniformly at random for the flea to jump to. The transition probabilities are

$$P_{ij} = \begin{cases} i/(2N), & \text{if } j = i-1, \\ (N-i)/(2N), & \text{if } j = i+1, \\ 1/2, & \text{if } j = i, \\ 0, & \text{otherwise.} \end{cases}$$

Since $P_{ii} > 0$, the chain is aperiodic, and thus ergodic. The unique stationary distribution is binomial with parameters N and $1/2$, the same as in the regular Ehrenfest scheme. (We invite the reader to show this in Exercise 3.24.) By the fundamental limit theorem, the stationary distribution is the limiting distribution of the chain. The long-term stationary process can be simply described: for each of the N fleas, toss a fair coin. If heads, the flea jumps to Lisa, if tails it jumps to Cooper.

The modified Ehrenfest transition matrix for $N = 6$ fleas is

$$\boldsymbol{P} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{array}{c} \begin{array}{ccccccc} 0 & 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{pmatrix} 1/2 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 5/12 & 1/2 & 1/12 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & 1/2 & 1/6 & 0 & 0 & 0 \\ 0 & 0 & 1/4 & 1/2 & 1/4 & 0 & 0 \\ 0 & 0 & 0 & 1/6 & 1/2 & 1/3 & 0 \\ 0 & 0 & 0 & 0 & 1/12 & 1/2 & 5/12 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 \end{pmatrix} \end{array},$$

with limiting distribution

$$\boldsymbol{\pi} = \left(\frac{1}{64}, \frac{6}{64}, \frac{15}{64}, \frac{20}{64}, \frac{15}{64}, \frac{6}{64}, \frac{1}{64} \right).$$

■

Example 3.20 Consider a Markov chain with transition matrix

$$
\boldsymbol{P} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ \vdots \\ \text{n-1} \\ \text{n} \end{array}
\begin{array}{c}
\begin{array}{ccccccc} 1 & 2 & 3 & 4 & \cdots & \text{n-1} & \text{n} \end{array} \\
\begin{pmatrix}
0 & 1 & 0 & 0 & \cdots & 0 & 0 \\
1/2 & 0 & 1/2 & 0 & \cdots & 0 & 0 \\
1/3 & 0 & 0 & 2/3 & \cdots & 0 & 0 \\
1/4 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
1/(n-1) & 0 & 0 & 0 & \cdots & 0 & (n-2)/(n-1) \\
1 & 0 & 0 & 0 & \cdots & 0 & 0
\end{pmatrix}
\end{array}.
$$

The transition graph is shown in Figure 3.9. Find the limiting distribution.

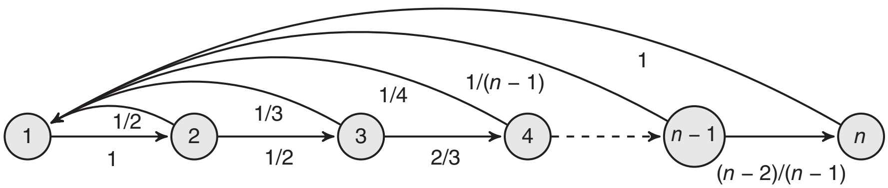

Figure 3.9

Solution State 1 is accessible from all states. Each state k is accessible from 1 by transitioning to 2, then 3, …, to k. Thus, the chain is irreducible. It is also aperiodic for $n \geq 3$. For instance, one can reach state 1 from 1 in either two steps or three steps. Thus, $d(1) = 1$. The chain is ergodic, and the limiting distribution is gotten by finding the stationary distribution.

Let $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$, with $x_1 = 1$. Solving

$$x_j = \sum_{i=1}^{n} x_i P_{ij} = x_{j-1} P_{j-1,j}, \text{ for } j = 2, \dots, n,$$

gives $x_2 = x_1 = 1$ and

$$
\begin{aligned}
x_j &= x_{j-1}\left(\frac{j-2}{j-1}\right) = x_{j-2}\left(\frac{j-3}{j-2}\right)\left(\frac{j-2}{j-1}\right) \\
&= x_{j-2}\left(\frac{j-3}{j-1}\right) = \cdots = x_2\left(\frac{1}{j-1}\right) = \frac{1}{j-1}, \text{ for } j = 3, \dots, n.
\end{aligned}
$$

Hence,

$$
\pi_j = \begin{cases} \dfrac{1}{c}, & \text{for } j = 1, \\ \dfrac{1}{c(j-1)}, & \text{for } j = 2, \dots, n, \end{cases}
$$

where $c = 1 + \sum_{k=1}^{n-1} 1/k$.

An infinite version of this chain—see Exercise 3.27—does not have a stationary distribution. Although the chain is aperiodic and irreducible, it is not positive recurrent. That is, the expected return time between visits to the same state is infinite.

■

Example 3.21 (PageRank) Google's PageRank search algorithm is introduced in Chapter 1 in Example 1.1. The model is based on the *random surfer* model, which is a random walk on the *webgraph*. For this graph, each vertex represents an internet page. A directed edge connects i to j if there is a hypertext link from page i to page j. When the random surfer is at page i, they move to a new page by choosing from the available links on i uniformly at random.

Figure 3.10 shows a simplified network with seven pages. The network is described by the *network matrix*

$$
\boldsymbol{N} = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \\ f \\ g \end{array}
\begin{array}{c}
\begin{array}{ccccccc} a & b & c & d & e & f & g \end{array} \\
\begin{pmatrix}
0 & 0 & 0 & 0 & 1/2 & 1/2 & 0 \\
1/3 & 0 & 1/3 & 0 & 0 & 1/3 & 0 \\
0 & 0 & 0 & 1/2 & 0 & 1/2 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
1/4 & 0 & 0 & 1/4 & 0 & 1/4 & 1/4 \\
1/2 & 1/2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\end{array}.
$$

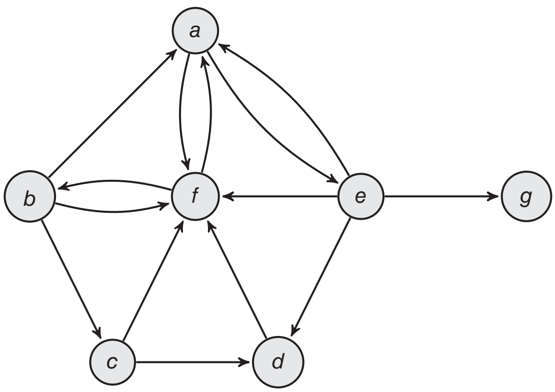

Figure 3.10

Note that $\boldsymbol{N}$ is not a stochastic matrix, as page g has no out-link. Row g consists of all 0s.

To insure that the walk reaches all pages in the network, the algorithm needs to account for (i) pages that have no out-links, called *dangling nodes*, and (ii) groups of pages that might result in the walk getting stuck in a subgraph. In the example network, node g is a dangling node.

Assume that the webgraph consists of k pages. In the PageRank algorithm, the fix for dangling nodes is to assume that when the random surfer reaches such a page they jump to a new page in the network uniformly at random. A new matrix $\boldsymbol{Q}$ is obtained where each row in the network matrix $\boldsymbol{N}$ corresponding to a dangling node is changed to one in which all entries are $1/k$. The matrix $\boldsymbol{Q}$ is a stochastic matrix.

For the problem of potentially getting stuck in small subgraphs of the webgraph, the solution proposed in the original paper by Brin and Page (1998) was to fix a *damping factor* $0 < p < 1$ for modifying the $\boldsymbol{Q}$ matrix. In their model, from a given page the random surfer, with probability $1 - p$, decides to not follow any links on the page and instead navigate to a new random page on the network. On the other hand, with probability p, they follow the links on the page as usual. This defines the PageRank transition matrix

$$\boldsymbol{P} = p\boldsymbol{Q} + (1 - p)\boldsymbol{A},$$

where $\boldsymbol{A}$ is a $k \times k$ matrix all of whose entries are $1/k$. The damping factor used by Google was originally set to $p = 0.85$.

With damping factor, the PageRank matrix $\boldsymbol{P}$ is stochastic, and the resulting random walk is aperiodic and irreducible. The PageRank of a page on the network is that page's stationary probability.

Consider the sample network in Figure 3.10. See the following `R` code for the relevant calculations. The PageRank stationary distribution is

a	b	c	d	e	f	g
0.222	0.153	0.071	0.084	0.122	0.294	0.054

Assume that you are searching this network with the query "stochastic process," and the search terms are found on pages a, c, e, and f. Ordered by their stationary probabilities, the PageRank algorithm would return the ordered pages f, a, e, c.

R: PageRank

```
# pagerank.R
> Q
       a      b      c      d      e      f      g
a 0.0000 0.0000 0.0000 0.0000 0.5000 0.5000 0.0000
b 0.3333 0.0000 0.3333 0.0000 0.0000 0.3333 0.0000
c 0.0000 0.0000 0.0000 0.5000 0.0000 0.5000 0.0000
d 0.0000 0.0000 0.0000 0.0000 0.0000 1.0000 0.0000
e 0.2500 0.0000 0.0000 0.2500 0.0000 0.2500 0.2500
f 0.5000 0.5000 0.0000 0.0000 0.0000 0.0000 0.0000
g 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429
> A <- matrix(rep(1/7,49),nrow=7)
```

```
> A
       a      b      c      d      e      f      g
a 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429
b 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429
c 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429
d 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429
e 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429
f 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429
g 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429 0.1429
# Transition matrix with damping factor p=0.85
> P <- 0.85*Q + 0.15*A
> pr <- stationary(P)
> pr  # Stationary probabilities
     a      b      c      d      e      f      g
0.2220 0.1527 0.0713 0.0843 0.1223 0.2935 0.0540
```

■

3.7 TIME REVERSIBILITY

Some Markov chains exhibit a directional bias in their evolution. Take, for instance, simple random walk on the integers, which moves from i to $i+1$ with probability p, and from i to $i-1$ with probability $1-p$. If $p > 1/2$, the walk tends to move in the positive direction, mostly hitting ever larger integers. Similarly, if $p < 1/2$, over time the chain tends to hit ever smaller integers. However, if $p = 1/2$, the chain exhibits no directional bias.

The property of time reversibility can be explained intuitively as follows. If you were to take a movie of the Markov chain moving forward in time and then run the movie backwards, you could not tell the difference between the two.

Time Reversibility

An irreducible Markov chain with transition matrix $\boldsymbol{P}$ and stationary distribution $\boldsymbol{\pi}$ is *reversible*, or *time reversible*, if

$$\pi_i P_{ij} = \pi_j P_{ji}, \text{ for all } i, j. \tag{3.8}$$

Equations (3.8) are called the *detailed balance equations*. They say that for a chain in stationarity,

$$P(X_0 = i, X_1 = j) = P(X_0 = j, X_1 = i), \text{ for all } i, j.$$

That is, the frequency of transitions from i to j is equal to the frequency of transitions from j to i.

More generally (see Exercise 3.39), if a stationary Markov chain is reversible then

$$P(X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n) = P(X_0 = i_n, X_1 = i_{n-1}, \ldots, X_n = i_0),$$

for all $i_0, i_1, \ldots, i_n$.

Example 3.22 A Markov chain has transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{pmatrix} 0 & 2/5 & 3/5 \\ 1/2 & 1/4 & 1/4 \\ 1/2 & 1/6 & 1/3 \end{pmatrix} \end{array}.$$

Determine if the chain is reversible.

Solution The chain is irreducible and aperiodic. The stationary distribution is $\boldsymbol{\pi} = (1/3, 4/15, 2/5)$. We check the detailed balance equations

$$\pi_1 P_{12} = \left(\frac{1}{3}\right)\left(\frac{2}{5}\right) = \frac{2}{15} = \left(\frac{4}{15}\right)\left(\frac{1}{2}\right) = \pi_2 P_{21},$$

$$\pi_1 P_{13} = \left(\frac{1}{3}\right)\left(\frac{3}{5}\right) = \frac{1}{5} = \left(\frac{2}{5}\right)\left(\frac{1}{2}\right) = \pi_3 P_{31},$$

and

$$\pi_2 P_{23} = \left(\frac{4}{15}\right)\left(\frac{1}{4}\right) = \frac{1}{15} = \left(\frac{2}{5}\right)\left(\frac{1}{6}\right) = \pi_3 P_{32}.$$

Thus, the chain is time reversible.

■

If the stationary distribution of a Markov chain is uniform, it is apparent from Equation (3.8) that the chain is reversible if the transition matrix is symmetric.

Example 3.23 Consider random walk on the n-cycle with transition matrix

$$\boldsymbol{P} = \begin{cases} p, & \text{if } j \equiv i+1 \mod n, \\ 1-p, & \text{if } j \equiv i-1 \mod n, \\ 0, & \text{otherwise.} \end{cases}$$

The stationary distribution is uniform. Hence, the random walk is time reversible for $p = 1/2$. For $p \neq 1/2$, directional bias of the walk will be apparent. For instance, if $p > 1/2$, the frequency of transitions from i to $i+1$ is greater than the frequency of transitions from $i+1$ to i. ■

Example 3.24 Simple random walk on a graph is time reversible. If i and j are neighbors, then

$$\pi_i P_{ij} = \left(\frac{\deg(i)}{2e}\right)\left(\frac{1}{\deg(i)}\right) = \frac{1}{2e} = \left(\frac{\deg(j)}{2e}\right)\left(\frac{1}{\deg(j)}\right) = \pi_j P_{ji}.$$

If i and j are not neighbors, $P_{ij} = P_{ji} = 0$. ■

Reversible Markov Chains and Random Walk on Weighted Graphs

Random walk on a weighted graph is time reversible. In fact, every reversible Markov chain can be considered as a random walk on a weighted graph.

Given a reversible Markov chain with transition matrix $\boldsymbol{P}$ and stationary distribution $\boldsymbol{\pi}$, construct a weighted graph on the state space by assigning edge weights $w(i,j) = \pi_i P_{ij}$. With these choice of weights, random walk on the weighted graph moves from i to j with probability

$$\frac{w(i,j)}{\sum_v w(i,v)} = \frac{\pi_i P_{ij}}{\sum_v \pi_i P_{iv}} = \frac{\pi_i P_{ij}}{\pi_i} = P_{ij}.$$

Conversely, given a weighted graph with edge weight function $w(i,j)$, the transition matrix of the corresponding Markov chain is obtained by letting

$$P_{ij} = \frac{w(i,j)}{\sum_v w(i,v)},$$

where the sum is over all neighbors of i. The stationary distribution is

$$\pi_i = \frac{\sum_y w(i,y)}{\sum_x \sum_y w(x,y)}.$$

One checks that

$$\begin{aligned}\pi_i P_{ij} &= \left(\frac{\sum_y w(i,y)}{\sum_x \sum_y w(x,y)}\right) \frac{w(i,j)}{\sum_y w(i,y)}\\ &= \frac{w(i,j)}{\sum_x \sum_y w(x,y)}\\ &= \left(\frac{\sum_y w(j,y)}{\sum_x \sum_y w(x,y)}\right) \frac{w(i,j)}{\sum_y w(j,y)} = \pi_j P_{ji}.\end{aligned}$$

Thus, the chain is time reversible.

Example 3.25 A reversible Markov chain has transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{pmatrix} 0 & 4/5 & 1/5 & 0 \\ 4/6 & 1/6 & 1/6 & 0 \\ 1/4 & 1/4 & 0 & 1/2 \\ 0 & 0 & 2/3 & 1/3 \end{pmatrix} \end{array}. \tag{3.9}$$

Find the associated weighted graph.

Solution The stationary distribution is found to be $\boldsymbol{\pi} = (5/18, 6/18, 4/18, 3/18)$. Arrange the quantities $\pi_i P_{ij}$ in a (nonstochastic) matrix

$$\boldsymbol{R} = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{pmatrix} 0 & 4/18 & 1/18 & 0 \\ 4/18 & 1/18 & 1/18 & 0 \\ 1/18 & 1/18 & 0 & 2/18 \\ 0 & 0 & 2/18 & 1/18 \end{pmatrix} \end{array},$$

where $R_{ij} = w(i,j) = \pi_i P_{ij}$. The matrix is symmetric. Multiplying the entries by 18 so that all weights are integers gives the weighted graph in Figure 3.11. ■

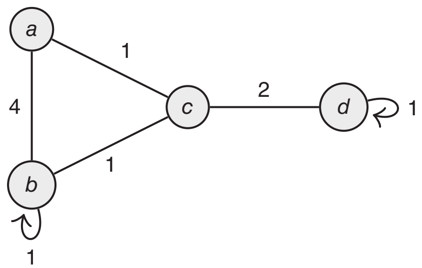

Figure 3.11 Weighted graph.

The next proposition highlights a key benefit of reversibility. It is often used to simplify computations for finding the stationary distribution of a Markov chain.

Proposition 3.9. *Let* $\boldsymbol{P}$ *be the transition matrix of a Markov chain. If* $\boldsymbol{x}$ *is a probability distribution which satisfies*

$$x_i P_{ij} = x_j P_{ji}, \textit{for all } i, j, \tag{3.10}$$

then $\boldsymbol{x}$ *is the stationary distribution, and the Markov chain is reversible.*

Proof. Assume that $\boldsymbol{x}$ satisfies the detailed balance equations. We have to show that $\boldsymbol{x} = \boldsymbol{xP}$. For all j,

$$(xP)_j = \sum_i x_i P_{ij} = \sum_i x_j P_{ji} = x_j.$$

■

Example 3.26 (Birth-and-death chain) Birth-and-death chains were introduced in Example 2.9. From i, the process moves to either $i-1$, i, or $i+1$, with respective probabilities q_i, $1-p_i-q_i$, and p_i. Show that a birth-and-death chain is time reversible and find the stationary distribution.

Solution To use Proposition 3.9, consider a vector $\boldsymbol{x}$ which satisfies the detailed balance equations. Then,

$$x_i P_{i,i+1} = x_{i+1} P_{i+1,i}, \text{ for } \quad i = 0, 1, \dots$$

giving

$$x_i p_i = x_{i+1} q_{i+1}, \text{ for } \quad i = 0, 1, \dots$$

Let $x_0 = 1$. Then, $x_1 = p_0/q_1$. Also, $x_2 = x_1 p_1/q_2 = (p_0 p_1)/(q_2 q_1)$. The general pattern is

$$x_k = \frac{p_0 p_1 \cdots p_{k-1}}{q_1 q_2 \cdots q_k} = \prod_{i=1}^{k} \frac{p_{i-1}}{q_i}, \text{ for } \quad k = 0, 1, \dots$$

Normalizing gives the stationary distribution

$$\pi_k = \frac{x_k}{\sum_j x_j},$$

assuming that the infinite sum $\sum_j x_j$ converges. Thus, a necessary condition for a stationary distribution to exist, in which case the birth-and-death chain is time reversible, is that

$$\sum_j \prod_{i=1}^{j} \frac{p_{i-1}}{q_i} < \infty.$$

Birth-and-death chains encompass a large variety of special models. For instance, *random walk with a partially reflecting boundary* on $\{0, 1, \dots, N\}$ is achieved as a birth-and-death chain by letting $p_i = p$ and $q_i = q$, for $0 \le i \le N$, with $p + q < 1$. See Figure 3.12.

Minor modification to this derivation gives the stationary probabilities

$$\pi_k = \frac{x_k}{\sum_{i=0}^{N} x_i}, \text{for} \quad k = 0, 1, \dots, N,$$

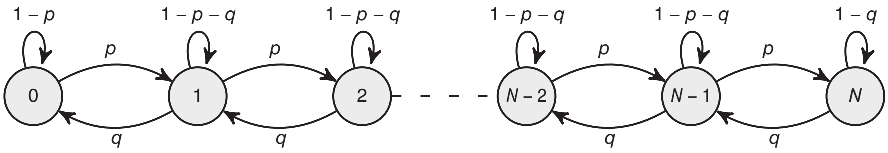

Figure 3.12 Random walk with partially reflecting boundaries.

where

$$x_k = \prod_{i=1}^{k} \left(\frac{p}{q}\right) = \left(\frac{p}{q}\right)^k, \text{ for } k = 0, 1, \ldots, N.$$

For $p \neq q$, this gives

$$\pi_k = \left(1 - \frac{p}{q}\right) \left(\frac{p}{q}\right)^k \Big/ \left(1 - \left(\frac{p}{q}\right)^{N+1}\right), \quad \text{for} \quad k = 0, 1, \ldots, N.$$

For $p = q$, the stationary distribution is uniform. ∎

3.8 ABSORBING CHAINS

Many popular board games can be modeled as Markov chains. The children's game *Chutes and Ladders* is based on an ancient Indian game called *Snakes and Ladders*. It is played on a 100-square board, as in Figure 3.13. Players each have a token and take turns rolling a six-sided die and moving their token by the corresponding number of squares. If a player lands on a *ladder*, they immediately move up the ladder to a higher-numbered square. If they move on a *chute*, or *snake*, they drop down to a lower-numbered square. The finishing square 100 must be reached by an exact roll of the die (or by landing on square 80 whose ladder climbs to the finish). The first player to land on square 100 wins.

The game is a Markov chain since the player's position only depends on their previous position and the roll of the die. The chain has 101 states as the game starts with all players off the board (state 0). For the Markov model, once the chain hits state 100 it stays at 100. That is, if $\boldsymbol{P}$ is the transition matrix, then $P_{100,100} = 1$.

Of particular interest is the average number of plays needed to reach the finish. The `R` script file **snakes.R** contains code for building the 101×101 transition matrix $\boldsymbol{P}$. Here are the results from several simulations of the game.

R: Snakes and Ladders

```
> init <- c(1,rep(0,100)) # Start at square 0
> markov(init,P,150,0:100)
  [1]   0   6  11  12   6  12  15  20  42  43  44  45  46  47  26
 [16]  29  33  37  40  42  44  47  52  55  57  60  61  19  22  24
```

```
 [31]   30  44  11  17  42  45  46  50  52  53  53  53  54  60  61
 [46]   63  65  68  73  77  78  82  86  92  94  99 100
 > markov(init,P,150,0:100)
  [1]    0  14  18  24  30  34  40  44  45  67  70  74 100
> markov(init,P,150,0:100)
  [1]    0   5   6   8  31  33  44  46  50  53  55  58  63  60  61
 [16]   66  72  77  78 100
 > markov(init,P,150,0:100)
  [1]    0   2   5   8  11  14  20  26  31  37  39  40  42  47  53
 [16]   58  63  60  60  65  69  72  76  82  86  24  25  29  31  35
 [31]   40  42  26  31  34  35  39  43  45  11  13  19  24  26  32
 [46]   35  38  39  42  44  26  84  88  90  96 100
 > markov(init,P,150,0:100)
  [1]    0   6  31  44  45  26  27  32  38  44  26  30  31  33  44
 [16]   46  50  67  73  76  77  78  79  84  88  90  73  76 100
 > markov(init,P,150,0:100)
  [1]    0   3  31  34  40  42  47  26  30  32  38  44  47  53  59
 [16]   19  23  25  31  44  26  29  31  33  37  41  42  26  31  32
 [31]   38  43  44  50  52  58  19  24  30  31  35  41  44  46  67
 [46]   68  91  97  99  99  99  99  99  99  99  99  99 100
 > markov(init,P,150,0:100)
  [1]    0   2   7  13   6  10  15  17  23  25  31  37  40  45  11
 [16]   17  20  26  31  33  44  46  26  29  35  44  50  67  72  74
 [31]   76 100
```

For these simulations, it took, respectively, 56, 12, 19, 55, 28, 57, and 31 steps to reach the winning square, for an average of 36.86 steps to win.

An exact analysis of the average time to win the game is given in this section, after establishing some theory.

In the Snakes and Ladders Markov chain every state, except 100, is transient. State 100 is recurrent. From 100, the chain stays at 100 forever. A state with this property is called *absorbing*.

Absorbing State, Absorbing Chain

State i is an *absorbing state* if $P_{ii} = 1$. A Markov chain is called an *absorbing chain* if it has at least one absorbing state.

Consider an absorbing Markov chain on k states for which t states are transient and $k - t$ states are absorbing. The states can be reordered, as in the canonical decomposition, with the transition matrix written in block matrix form

$$\boldsymbol{P} = \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right) \tag{3.11}$$

where $\boldsymbol{Q}$ is a $t \times t$ matrix, $\boldsymbol{R}$ is a $t \times (k - t)$ matrix, $\boldsymbol{0}$ is a $(k - t) \times t$ matrix of 0s, and $\boldsymbol{I}$ is the $(k - t) \times (k - t)$ identity matrix.

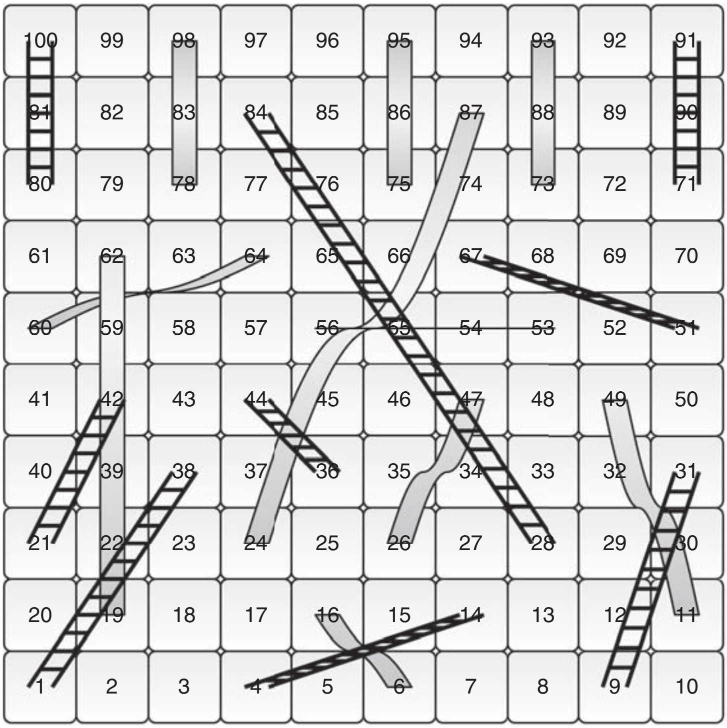

Figure 3.13 Children's Snakes and Ladders game. Board drawn using Ti*k*Z TeX package. *Source*: http://tex.stackexchange.com/questions/85411/chutes-and-ladders/. Reproduced with permission of Serge Ballif.

Computing powers of $\boldsymbol{P}$ is facilitated by the block matrix form. We have

$$\boldsymbol{P}^2 = \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right)\left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right) = \left(\begin{array}{c|c} \boldsymbol{Q}^2 & (\boldsymbol{I}+\boldsymbol{Q})\boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right),$$

$$\boldsymbol{P}^3 = \left(\begin{array}{c|c} \boldsymbol{Q}^3 & (\boldsymbol{I}+\boldsymbol{Q}+\boldsymbol{Q}^2)\boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right),$$

and, in general,

$$\boldsymbol{P}^n = \left(\begin{array}{c|c} \boldsymbol{Q}^n & (\boldsymbol{I}+\boldsymbol{Q}+\cdots+\boldsymbol{Q}^{n-1})\boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right), \quad \text{for } n \geq 1. \tag{3.12}$$

To find the limiting matrix $\lim_{n\to\infty} \boldsymbol{P}^n$, we make use of the following lemma from linear algebra.

Lemma 3.10. *Let* $\boldsymbol{A}$ *be a square matrix with the property that* $\boldsymbol{A}^n \to \boldsymbol{0}$*, as* $n \to \infty$*. Then,*

$$\sum_{n=0}^{\infty} \boldsymbol{A}^n = (\boldsymbol{I} - \boldsymbol{A})^{-1}.$$

The lemma gives the matrix analog of the sum of a geometric series of real numbers. That is,

$$\sum_{n=0}^{\infty} r^n = (1 - r)^{-1},$$

if $r^n \to 0$, as $n \to \infty$.

Proof. For fixed n,

$$\begin{aligned}(\boldsymbol{I} - \boldsymbol{A})(\boldsymbol{I} + \boldsymbol{A} + \boldsymbol{A}^2 + \cdots + \boldsymbol{A}^n) &= \boldsymbol{I} + \boldsymbol{A} + \boldsymbol{A}^2 + \cdots + \boldsymbol{A}^n \\ &\quad - (\boldsymbol{A} + \boldsymbol{A}^2 + \cdots + \boldsymbol{A}^n + \boldsymbol{A}^{n+1}) \\ &= \boldsymbol{I} - \boldsymbol{A}^{n+1}.\end{aligned}$$

If $\boldsymbol{I} - \boldsymbol{A}$ is invertible, then

$$(\boldsymbol{I} + \boldsymbol{A} + \cdots + \boldsymbol{A}^n) = (\boldsymbol{I} - \boldsymbol{A})^{-1}(\boldsymbol{I} - \boldsymbol{A}^{n+1}).$$

Taking limits, as $n \to \infty$, gives

$$\sum_{n=0}^{\infty} \boldsymbol{A}^n = (\boldsymbol{I} - \boldsymbol{A})^{-1},$$

since $\boldsymbol{A}^{n+1} \to \boldsymbol{0}$, as $n \to \infty$.

To show that $\boldsymbol{I} - \boldsymbol{A}$ is invertible, consider the linear system $(\boldsymbol{I} - \boldsymbol{A})\boldsymbol{x} = \boldsymbol{0}$. Invertibility of $\boldsymbol{I} - \boldsymbol{A}$ is equivalent to the fact that the only solution to this system is $\boldsymbol{x} = \boldsymbol{0}$. We have that $\boldsymbol{0} = (\boldsymbol{I} - \boldsymbol{A})\boldsymbol{x} = \boldsymbol{x} - \boldsymbol{A}\boldsymbol{x}$. That is, $\boldsymbol{x} = \boldsymbol{A}\boldsymbol{x}$. Iterating gives

$$\boldsymbol{x} = \boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}(\boldsymbol{A}\boldsymbol{x}) = \boldsymbol{A}^2\boldsymbol{x} = \cdots = \boldsymbol{A}^n\boldsymbol{x}, \text{ for all } n \geq 1.$$

Taking limits on both sides of the equation gives

$$\boldsymbol{x} = \lim_{n\to\infty} \boldsymbol{A}^n\boldsymbol{x} = \boldsymbol{0}.$$ ■

To apply Lemma 3.10 to Equation (3.12), observe that $\boldsymbol{Q}^n \to \boldsymbol{0}$, as $n \to \infty$. The matrix $\boldsymbol{Q}$ is indexed by transient states. If i and j are transient,

$$\lim_{n\to\infty} Q_{ij}^n = \lim_{n\to\infty} P_{ij}^n = 0,$$

as the long-term probability that a Markov chain hits a transient state is 0. Taking limits in Equation (3.12) gives

$$\lim_{n\to\infty} \boldsymbol{P}^n = \lim_{n\to\infty} \left(\begin{array}{c|c} \boldsymbol{Q}^n & (\boldsymbol{I}+\boldsymbol{Q}+\cdots+\boldsymbol{Q}^{n-1})\boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right)$$
$$= \left(\begin{array}{c|c} \lim_{n\to\infty} \boldsymbol{Q}^n & \lim_{n\to\infty}(\boldsymbol{I}+\boldsymbol{Q}+\cdots+\boldsymbol{Q}^{n-1})\boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right)$$
$$= \left(\begin{array}{c|c} \boldsymbol{0} & (\boldsymbol{I}-\boldsymbol{Q})^{-1}\boldsymbol{R} \\ \hline \boldsymbol{0} & \boldsymbol{I} \end{array}\right).$$

Consider the interpretation of the limiting submatrix $(\boldsymbol{I}-\boldsymbol{Q})^{-1}\boldsymbol{R}$. The matrix is indexed by transient rows and absorbing columns. The ijth entry is the long-term probability that the chain started in transient state i is absorbed in state j. If the Markov chain has only one absorbing state, this submatrix will be a $(k-1)$-element column vector of 1s.

Example 3.27 (Gambler's ruin) A gambler starts with \$2 and plays a game where the chance of winning each round is 60%. The gambler either wins or loses \$1 on each round. The game stops when the gambler either gains \$5 or goes bust. Find the probability that the gambler is eventually ruined.

Solution The game is an absorbing Markov chain with absorbing states 0 and 5. The transition matrix in canonical form is

$$\boldsymbol{P} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 0 \\ 5 \end{array} \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & 0 & 5 \end{array} \\ \begin{pmatrix} 0 & 0.6 & 0 & 0 & 0.4 & 0 \\ 0.4 & 0 & 0.6 & 0 & 0 & 0 \\ 0 & 0.4 & 0 & 0.6 & 0 & 0 \\ 0 & 0 & 0.4 & 0 & 0 & 0.6 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array},$$

with

$$\boldsymbol{Q} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 0 & 0.6 & 0 & 0 \\ 0.4 & 0 & 0.6 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0 & 0.4 & 0 \end{pmatrix} \end{array} \quad \text{and} \quad \boldsymbol{R} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cc} 0 & 5 \end{array} \\ \begin{pmatrix} 0.4 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0.6 \end{pmatrix} \end{array}.$$

This gives

$$(\boldsymbol{I}-\boldsymbol{Q})^{-1}\boldsymbol{R} = \begin{pmatrix} 1 & -0.6 & 0 & 0 \\ -0.4 & 1 & -0.6 & 0 \\ 0 & -0.4 & 1 & -0.6 \\ 0 & 0 & -0.4 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 0.4 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0.6 \end{pmatrix}$$

$$= \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cc} 0 & \quad 5 \end{array} \\ \begin{pmatrix} 0.616 & 0.384 \\ 0.360 & 0.640 \\ 0.190 & 0.810 \\ 0.076 & 0.924 \end{pmatrix} \end{array}.$$

If the gambler starts with \$2, the probability of their eventual ruin is 0.36.

`R`: Gambler's Ruin

Commands for working with matrices in `R` are explained in Appendix E. The `R` command `solve(mat)` computes the matrix inverse of `mat`. The command `diag(k)` generates a $k \times k$ identity matrix.

```
> P
    1   2   3   4   0   5
1 0.0 0.6 0.0 0.0 0.4 0.0
2 0.4 0.0 0.6 0.0 0.0 0.0
3 0.0 0.4 0.0 0.6 0.0 0.0
4 0.0 0.0 0.4 0.0 0.0 0.6
0 0.0 0.0 0.0 0.0 1.0 0.0
5 0.0 0.0 0.0 0.0 0.0 1.0
> Q <- P[1:4,1:4]
> R <- P[1:4,5:6]
> Q
    1   2   3   4
1 0.0 0.6 0.0 0.0
2 0.4 0.0 0.6 0.0
3 0.0 0.4 0.0 0.6
4 0.0 0.0 0.4 0.0
> R
    0   5
1 0.4 0.0
2 0.0 0.0
3 0.0 0.0
4 0.0 0.6
```

```
> solve(diag(4)-Q) %*% R
          0       5
1 0.616114 0.38389
2 0.360190 0.63981
3 0.189573 0.81043
4 0.075829 0.92417
```

■

For absorbing Markov chains, the matrix $(\boldsymbol{I}-\boldsymbol{Q})^{-1}$ is called the *fundamental matrix*. Its importance is highlighted by the next theorem. Recall that if i is transient, then for the chain started in i, the expected number of visits to i is finite.

Expected Number of Visits to Transient States

Theorem 3.11. *Consider an absorbing Markov chain with t transient states. Let $\boldsymbol{F}$ be a $t \times t$ matrix indexed by transient states, where F_{ij} is the expected number of visits to j given that the chain starts in i. Then,*

$$\boldsymbol{F} = (\boldsymbol{I}-\boldsymbol{Q})^{-1}.$$

Two proofs are given. The first uses the method of first-step analysis.

Proof #1. Let T be the set of transient states. Assume that $i, j \in T$. Consider the chain started in i. On the first step, the chain moves to some state k. If k is an absorbing state, then the chain will never visit j, unless $j = i$, in which case it has visited j one time. If k is a transient state, then the expected number of visits to j is F_{kj}, if $j \neq i$, and $1 + F_{ki}$, if $j = i$. This gives

$$\begin{aligned}
F_{ij} &= \begin{cases} \sum_{k\in T} P_{ik}(1+F_{ki}) + \sum_{k\notin T} P_{ik}, & \text{if } j = i,\\ \sum_{k\in T} P_{ik}F_{kj}, & \text{if } j \neq i,\end{cases}\\
&= \begin{cases} 1 + \sum\limits_{k\in T} Q_{ik}F_{ki}, & \text{if } j = i,\\ \sum_{k\in T} Q_{ik}F_{kj}, & \text{if } j \neq i,\end{cases}\\
&= \delta_{ij} + \sum_{k\in T} Q_{ik}F_{kj}, \qquad (3.13)
\end{aligned}$$

where $\delta_{ij} = 1$, if $i = j$, and 0, otherwise. The second equality is because if i and k are transient states, then $P_{ik} = Q_{ik}$.

In matrix terms, Equation (3.13) says that $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{QF}$, or $(\boldsymbol{I}-\boldsymbol{Q})\boldsymbol{F} = \boldsymbol{I}$. It follows that $\boldsymbol{I}-\boldsymbol{Q}$ is invertible and $(\boldsymbol{I}-\boldsymbol{Q})^{-1} = \boldsymbol{F}$. ■

Proof #2. For the chain started in i, define indicator variables

$$I_n = \begin{cases} 1, & \text{if } X_n = j, \\ 0, & \text{otherwise,} \end{cases}$$

for $n = 0, 1, \ldots$ Then, $\sum_{n=0}^{\infty} I_n$ is the number of visits to j. The expected number of visits is

$$\begin{aligned} F_{ij} &= E\left(\sum_{n=0}^{\infty} I_n\right) = \sum_{n=0}^{\infty} E(I_n) \\ &= \sum_{n=0}^{\infty} P(X_n = j | X_0 = i) \\ &= \sum_{n=0}^{\infty} P_{ij}^n = \sum_{n=0}^{\infty} Q_{ij}^n = \left(\sum_{n=0}^{\infty} Q^n\right)_{ij} = (I - Q)_{ij}^{-1}, \end{aligned}$$

as a consequence of Lemma 3.10. ∎

Expected Time to Absorption

For an absorbing Markov chain started in transient state i, let a_i be the expected absorption time, the expected number of steps to reach some absorbing state. The number of transitions from i to an absorbing state is simply the sum of the number of transitions from i to each of the transient states until eventual absorption. The expected number of steps from i to transient state j is F_{ij}. It follows that

$$a_i = \sum_{k \in T} F_{ik}.$$

In vector form, $\boldsymbol{a} = \boldsymbol{F1}$, where $\mathbf{1}$ is the column vector of all 1s. That is, the expected absorption times are the row sums of the fundamental matrix.

We summarize results for absorbing Markov chains.

Absorbing Markov Chains

For an absorbing Markov chain with all states either transient or absorbing, let $\boldsymbol{F} = (\boldsymbol{I} - \boldsymbol{Q})^{-1}$.

1. *(Absorption probability)* The probability that from transient state i the chain is absorbed in state j is $(FR)_{ij}$.
2. *(Absorption time)* The expected number of steps from transient state i until the chain is absorbed in some absorbing state is $(F1)_i$.

Example 3.28 (Snakes and Ladders) We find the expected absorption time to square 100 in Snakes and Ladders. See the **snakes.R** script file. The transition matrix is a 101×101 matrix stored in the variable `P`.

R: Snakes and Ladders

```
> Q <- P[1:100,1:100]
> F <- solve(diag(100)-Q)
> a <- F %*% rep(1,100) # Expected absorption times
> round(t(a),2)
    0     1     2     3     4     5     6     7     8     9
39.60 40.25 40.07 39.57 39.84 39.67 39.46 39.23 38.98 39.05
   10    11    12    13    14    15    16    17    18    19
39.11 38.64 38.22 37.84 37.50 37.02 36.08 35.82 35.66 35.55
   20    21    22    23    24    25    26    27    28    29
35.50 35.50 33.82 34.31 34.66 34.94 35.15 35.30 37.52 37.25
   30    31    32    33    34    35    36    37    38    39
36.77 36.60 36.41 36.19 35.93 35.64 35.68 35.55 35.31 34.83
   40    41    42    43    44    45    46    47    48    49
34.37 33.93 34.10 34.75 33.87 31.95 31.61 31.27 30.20 28.47
   50    51    52    53    54    55    56    57    58    59
28.58 29.88 29.61 29.22 28.75 28.24 29.29 28.28 27.94 26.87
   60    61    62    63    64    65    66    67    68    69
25.95 25.16 22.57 22.19 21.16 20.42 20.43 20.44 20.03 19.85
   70    71    72    73    74    75    76    77    78    79
19.81 20.50 20.50 20.52 17.59 18.74 19.56 20.12 20.47 20.64
   80    81    82    83    84    85    86    87    88    89
24.12 25.62 24.48 23.53 22.56 21.62 20.90 18.54 17.63 17.79
   90    91    92    93    94    95    96    97    98    99
16.79 15.94 16.59 14.17 12.14 10.82 10.82 10.82  6.00  6.00
```

The desired expectation is a_0. At the start of the game, it takes, on average, 39.60 moves to reach the ending square. ■

Example 3.29 (Graduation) Recall the graduation Markov chain of Example 2.19. Students at a 4-year college either drop out, repeat a year, or move on to the next year. The chain is an absorbing chain with graduating and dropping out as absorbing states. Relevant matrices are

$$
\boldsymbol{P} = \begin{array}{r} \\ \text{Fr} \\ \text{So} \\ \text{Jr} \\ \text{Se} \\ \text{Drop} \\ \text{Grad} \end{array} \begin{array}{c} \begin{array}{cccccc} \text{Fr} & \text{So} & \text{Jr} & \text{Sr} & \text{Drop} & \text{Grad} \end{array} \\ \begin{pmatrix} 0.03 & 0.91 & 0 & 0 & 0.06 & 0 \\ 0 & 0.03 & 0.91 & 0 & 0.06 & 0 \\ 0 & 0 & 0.03 & 0.93 & 0.04 & 0 \\ 0 & 0 & 0 & 0.03 & 0.04 & 0.93 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array},
$$

$$\boldsymbol{Q} = \begin{array}{c} \\ \text{Fr} \\ \text{So} \\ \text{Jr} \\ \text{Se} \end{array} \begin{array}{c} \begin{array}{cccc} \text{Fr} & \text{So} & \text{Jr} & \text{Sr} \end{array} \\ \begin{pmatrix} 0.03 & 0.91 & 0 & 0 \\ 0 & 0.03 & 0.91 & 0 \\ 0 & 0 & 0.03 & 0.93 \\ 0 & 0 & 0 & 0.03 \end{pmatrix} \end{array}, \quad \text{and } \boldsymbol{R} = \begin{array}{c} \\ \text{Fr} \\ \text{So} \\ \text{Jr} \\ \text{Se} \end{array} \begin{array}{c} \begin{array}{cc} \text{Drop} & \text{Grad} \end{array} \\ \begin{pmatrix} 0.06 & 0 \\ 0.06 & 0 \\ 0.04 & 0 \\ 0.04 & 0.93 \end{pmatrix} \end{array}.$$

This gives

$$(\boldsymbol{I} - \boldsymbol{Q})^{-1}\boldsymbol{R} = \begin{pmatrix} 0.97 & -0.91 & 0 & 0 \\ 0 & 0.97 & -0.91 & 0 \\ 0 & 0 & 0.97 & -0.93 \\ 0 & 0 & 0 & 0.97 \end{pmatrix}^{-1} \begin{pmatrix} 0.06 & 0 \\ 0.06 & 0 \\ 0.04 & 0 \\ 0.04 & 0.93 \end{pmatrix}$$

$$= \begin{array}{c} \\ \text{Fr} \\ \text{So} \\ \text{Jr} \\ \text{Se} \end{array} \begin{array}{c} \begin{array}{cc} \text{Drop} & \text{Grad} \end{array} \\ \begin{pmatrix} 0.191 & 0.809 \\ 0.138 & 0.862 \\ 0.081 & 0.919 \\ 0.041 & 0.959 \end{pmatrix} \end{array}.$$

For a student who starts as a first-year, the probability of eventually graduating is 0.809. ■

R: Graduation

```
> P
       Fr   So   Jr   Se Drop Grad
Fr   0.03 0.91 0.00 0.00 0.06 0.00
So   0.00 0.03 0.91 0.00 0.06 0.00
Jr   0.00 0.00 0.03 0.93 0.04 0.00
Se   0.00 0.00 0.00 0.03 0.04 0.93
Drop 0.00 0.00 0.00 0.00 1.00 0.00
Grad 0.00 0.00 0.00 0.00 0.00 1.00
> Q <- P[1:4,1:4]
> R <- P[1:4,5:6]
> Absorb <- solve(diag(4)-Q)%*% R
> Absorb
       Drop    Grad
Fr 0.190975 0.80902
So 0.137633 0.86237
Jr 0.080774 0.91923
Se 0.041237 0.95876
```

Expected Hitting Times for Irreducible Chains

For an irreducible Markov chain, first hitting times can be analyzed as absorption times for a suitably modified chain. In particular, assume that $\boldsymbol{P}$ is the transition matrix of an irreducible Markov chain. To find the expected time until state i is first hit, consider a new chain in which i is an absorbing state. The transition matrix $\widetilde{\boldsymbol{P}}$ for the new chain is gotten by zeroing out the ith row of the $\boldsymbol{P}$ matrix and setting $\widetilde{P}_{ii} = 1$. The resulting $\boldsymbol{Q}$ matrix is obtained from $\widetilde{\boldsymbol{P}}$ by deleting the ith row and the ith column of $\boldsymbol{P}$. The time that the original $\boldsymbol{P}$-chain first hits i is equal to the time that the modified $\widetilde{\boldsymbol{P}}$-chain is absorbed in i.

Example 3.30 Consider random walk on the weighted graph in Figure 3.14. Starting from each vertex in the graph, find the expected number of steps until the walk first hits f.

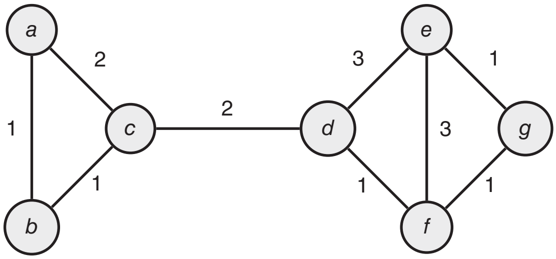

Figure 3.14

Solution The transition matrix is

$$\boldsymbol{P} = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \\ f \\ g \end{array} \begin{array}{c} \begin{array}{ccccccc} a & b & c & d & e & f & g \end{array} \\ \begin{pmatrix} 0 & 1/3 & 2/3 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 & 0 & 0 \\ 2/5 & 1/5 & 0 & 2/5 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 1/2 & 1/6 & 0 \\ 0 & 0 & 0 & 3/7 & 0 & 3/7 & 1/7 \\ 0 & 0 & 0 & 1/5 & 3/5 & 0 & 1/5 \\ 0 & 0 & 0 & 0 & 1/2 & 1/2 & 0 \end{pmatrix} \end{array}.$$

By making f an absorbing state, the resulting $\boldsymbol{Q}$ matrix is

$$\boldsymbol{Q} = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \\ g \end{array} \begin{array}{c} \begin{array}{cccccc} a & b & c & d & e & g \end{array} \\ \begin{pmatrix} 0 & 1/3 & 2/3 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 & 0 \\ 2/5 & 1/5 & 0 & 2/5 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 3/7 & 0 & 1/7 \\ 0 & 0 & 0 & 0 & 1/2 & 0 \end{pmatrix} \end{array},$$

which gives

$$F = (I - Q)^{-1} = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \\ g \end{array} \begin{array}{c} \begin{array}{cccccc} a & b & c & d & e & g \end{array} \\ \begin{pmatrix} 3.847 & 2.165 & 4.412 & 2.294 & 1.235 & 0.176 \\ 3.247 & 2.965 & 4.412 & 2.294 & 1.235 & 0.176 \\ 2.647 & 1.765 & 4.412 & 2.294 & 1.235 & 0.176 \\ 1.147 & 0.765 & 1.912 & 2.29 & 1.235 & 0.176 \\ 0.529 & 0.353 & 0.882 & 1.059 & 1.647 & 0.235 \\ 0.265 & 0.176 & 0.441 & 0.529 & 0.824 & 1.118 \end{pmatrix} \end{array}.$$

Row sums are

$$\begin{array}{c} a \\ b \\ c \\ d \\ e \\ g \end{array} \begin{pmatrix} 14.129 \\ 14.329 \\ 12.529 \\ 7.529 \\ 4.706 \\ 3.353 \end{pmatrix},$$

which gives the expected numbers of steps, starting from each vertex in the graph, to first hit f. ■

Example 3.31 A coin is flipped repeatedly until three heads in a row appear. What is the expected number of flips needed?

Solution One approach is to condition on the first coin flip and use the law of total expectation. Here is a Markov chain solution.

Let X_n be the most recent run of heads gotten after the nth coin flip. States are depicted as {Ø, H, HH, HHH}, with HHH an absorbing state and Ø representing the initial state. Note that if tails is ever flipped then the run of heads starts over again. Thus, Ø also represents having gotten tails on the last flip. The transition matrix is

$$P = \begin{array}{c} \\ Ø \\ \text{H} \\ \text{HH} \\ \text{HHH} \end{array} \begin{array}{c} \begin{array}{cccc} Ø & \text{H} & \text{HH} & \text{HHH} \end{array} \\ \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array}.$$

This gives

$$I - Q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & 1 \end{pmatrix}$$

and

$$F = (I - Q)^{-1} = \begin{pmatrix} 8 & 4 & 2 \\ 6 & 4 & 2 \\ 4 & 2 & 2 \end{pmatrix},$$

with expected absorption times

$$\boldsymbol{a} = \boldsymbol{F1} = \begin{array}{c} \\ \emptyset \\ \text{H} \\ \text{HH} \end{array} \begin{array}{c} \text{HHH} \\ \begin{pmatrix} 14 \\ 12 \\ 8 \end{pmatrix} \end{array}.$$

It takes on average 14 flips to get three heads in a row. ■

Patterns in Sequences

The last example illustrates a general method for problems involving the occurrence of patterns in random trials. Assume that the elements of a set S are repeatedly sampled. A *pattern* is a sequence $(p_1, p_2, \ldots, p_n)$, such that each of the p_i is an element of S. In the last example, $S = \{\text{H, T}\}$, and the desired pattern is (H,H,H).

For $k = 1, \ldots, n$, let $s_k = (p_1, \ldots, p_k)$ be the subsequence consisting of the first k elements of the pattern. A Markov chain is constructed with state space $\{\emptyset, s_1, \ldots, s_n\}$, where s_n, the desired pattern, is an absorbing state. The absorption time for the Markov chain is equal to the time until the pattern first appears in repeated sampling from S.

Example 3.32 A biased coin comes up heads, with probability 2/3, and tails, with probability 1/3. The coin is repeatedly flipped. How many flips are needed, on average, until the pattern HTHTH first appears?

Solution An absorbing Markov chain is constructed with transition matrix

$$\boldsymbol{P} = \begin{array}{l} \\ \emptyset \\ \text{H} \\ \text{HT} \\ \text{HTH} \\ \text{HTHT} \\ \text{HTHTH} \end{array} \begin{array}{c} \begin{array}{cccccc} \emptyset & \text{H} & \text{HT} & \text{HTH} & \text{HTHT} & \text{HTHTH} \end{array} \\ \begin{pmatrix} 1/3 & 2/3 & 0 & 0 & 0 & 0 \\ 0 & 2/3 & 1/3 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 2/3 & 0 & 0 \\ 0 & 2/3 & 0 & 0 & 1/3 & 0 \\ 1/3 & 0 & 0 & 0 & 0 & 2/3 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}.$$

The fundamental matrix is

$$\boldsymbol{F} = (\boldsymbol{I} - \boldsymbol{Q})^{-1} = \begin{pmatrix} 2/3 & -2/3 & 0 & 0 & 0 \\ 0 & 1/3 & -1/3 & 0 & 0 \\ -1/3 & 0 & 1 & -2/3 & 0 \\ 0 & -2/3 & 0 & 1 & -1/3 \\ -1/3 & 0 & 0 & 0 & 1 \end{pmatrix}^{-1}$$

$$= \begin{pmatrix} 45/8 & 81/4 & 27/4 & 9/2 & 3/2 \\ 33/8 & 81/4 & 27/4 & 9/2 & 3/2 \\ 33/8 & 69/4 & 27/4 & 9/2 & 3/2 \\ 27/8 & 63/4 & 21/4 & 9/2 & 3/2 \\ 15/8 & 27/4 & 9/4 & 3/2 & 3/2 \end{pmatrix}.$$

The sum of the first row of the fundamental matrix is

$$\frac{45}{8} + \frac{81}{4} + \frac{27}{4} + \frac{9}{2} + \frac{3}{2} = \frac{309}{8} = 38.625.$$

It takes, on average, 38.625 flips before HTHTH first appears. ■

R : Simulation of Number of Flips Needed For HTHTH

```
# pattern.R
# P(Heads) = 2/3, P(Tails) = 1/3
> trials <- 100000
> simlist <- numeric(trials)
> for (i in 1:trials) {
+ pattern <- c(1,0,1,0,1) # 1:Heads, 0:Tails
+ state <- sample(c(0,1),5,prob=c(1/3,2/3),replace=T)
+ k <- 5
+ while (!prod(state==pattern))
+  { flip <- sample(c(0,1),1,prob=c(1/3,2/3))
+  state <- c(tail(state,4),flip)
+  k <- k + 1 }
+  simlist[i] <- k }
>  mean(simlist)
[1] 38.67718
# exact expectation is 38.625
```

In the last example, successive trials (e.g., coin flips) are independent and identically distributed. However, this is not necessary. In the next example, the trials themselves form a Markov chain.

Example 3.33 Assume that successive occurrences of DNA nucleotides on a chromosome are modeled by a Markov chain with transition matrix

$$\widetilde{\boldsymbol{P}} = \begin{array}{c} \\ a \\ c \\ g \\ t \end{array} \begin{array}{c} \begin{array}{cccc} a & c & g & t \end{array} \\ \begin{pmatrix} 0.3 & 0.2 & 0.3 & 0.2 \\ 0.4 & 0.3 & 0.1 & 0.2 \\ 0.25 & 0.15 & 0.4 & 0.2 \\ 0.2 & 0.2 & 0.3 & 0.3 \end{pmatrix} \end{array}.$$

Consider searching sequentially across the chromosome until the pattern *accgc* first appears. On average, how many steps (e.g., successive nucleotides), are needed?

Solution An absorbing Markov chain is built on $\{\emptyset, a, ac, acc, accg, accgc\}$, with transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ \emptyset \\ a \\ ac \\ acc \\ accg \\ accgc \end{array} \begin{array}{c} \begin{array}{cccccc} \emptyset & a & ac & acc & accg & accgc \end{array} \\ \begin{pmatrix} 0.7 & 0.3 & 0 & 0 & 0 & 0 \\ 0.5 & 0.3 & 0.2 & 0 & 0 & 0 \\ 0.3 & 0.4 & 0 & 0.3 & 0 & 0 \\ 0.5 & 0.4 & 0 & 0 & 0.1 & 0 \\ 0.6 & 0.25 & 0 & 0 & 0 & 0.15 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}.$$

To understand the matrix entries, observe, for instance, that from state acc, the chain moves to (i) $accg$, with probability $\widetilde{P}_{cg} = 0.1$, or to (ii) a, with probability $\widetilde{P}_{ca} = 0.4$, or to (iii) $\emptyset$, with the complementary probability 0.5. We have

$$\begin{aligned} \boldsymbol{F} = (\boldsymbol{I} - \boldsymbol{Q})^{-1} &= \begin{pmatrix} 0.3 & -0.3 & 0 & 0 & 0 \\ -0.5 & 0.7 & -0.2 & 0 & 0 \\ -0.3 & -0.4 & 1 & -0.3 & 0 \\ -0.5 & -0.4 & 0 & 0.9 & 0 \\ -0.6 & -0.25 & 0 & 0 & 1 \end{pmatrix}^{-1} \\ &= \begin{pmatrix} 2201.85 & 1111.11 & 222.22 & 66.67 & 6.67 \\ 2198.52 & 1111.11 & 222.22 & 66.67 & 6.67 \\ 2190.19 & 1106.11 & 222.22 & 66.67 & 6.67 \\ 2167.41 & 1094.44 & 218.89 & 66.67 & 6.67 \\ 1870.74 & 944.444 & 188.89 & 56.67 & 6.67 \end{pmatrix}. \end{aligned}$$

The sum of the first row is

$$2201.85 + 1111.11 + 222.22 + 66.67 + 6.67 = 3608.52,$$

which gives the average number of nucleotides needed to reach the desired pattern. ■

3.9 REGENERATION AND THE STRONG MARKOV PROPERTY*

A Markov chain is sometimes observed from a fixed time $n > 0$ into the future. Assume that $X_0, X_1, \ldots$ is a Markov chain with transition matrix $\boldsymbol{P}$. Then, the process started at $n > 0$, $X_n, X_{n+1}, X_{n+2}, \ldots$ is also a Markov chain with transition matrix $\boldsymbol{P}$. This is a consequence of the Markov property, which says that given the present, past, and future are independent.

The *strong Markov property* asserts that for certain types of random times called *stopping times*, the Markov property holds. If S is a stopping time, then the sequence $X_S, X_{S+1}, X_{S+2}, \ldots$ is a Markov chain. Given that the present time is a stopping time, past and future are independent.

An integer-valued random variable S is a stopping time for a Markov chain if, for each s, the event $\{S = s\}$ can be determined from $X_0, \dots, X_s$. In other words, if the outcomes $X_0, \dots, X_s$ are known, then it can be determined whether or not $\{S = s\}$ occurs.

An important example of a stopping time is the *first hitting time* random variable

$$T_i = \min\{n \geq 0 : X_n = i\},$$

which is the first time that a Markov chain hits state i. For instance, consider the weather Markov chain. Let r denote rain. Then, T_r is the first day that it rains. For any day t, If we are given the succession of weather states up to time t, $X_0, \dots, X_t$, then it can be determined whether or not the first day that it rained was on day t. This shows that T_r is a stopping time. By the strong Markov property, the sequence $X_{T_r}, X_{T_r+1}, \dots$ is a Markov chain.

A closely related stopping time for a Markov chain started at i, is the *first return time*

$$T_i^+ = \min\{n \geq 1 : X_n = i\}.$$

The strong Markov property says that the chain started at T_i^+ looks the same as the chain started at i. We say that at time T_i^+ the Markov chain *regenerates itself* and probabilistically starts anew.

More generally, given a nonempty subset of states $A \subseteq \mathcal{S}$, the first time the chain hits a state in A

$$T_A = \min\{n \geq 0 : X_n \in A\}$$

is a stopping time.

A random time that is not a stopping time is the *last* visit to state i. Knowing whether or not the last visit to i occurs at time s cannot be determined from just $X_0, \dots, X_s$. It requires knowledge of the entire Markov sequence $X_0, X_1, \dots$

Strong Markov Property

Let $X_0, X_1, \dots$ be a Markov chain with transition matrix $\boldsymbol{P}$. Let S be a stopping time. Then, $X_S, X_{S+1}, \dots$ is a Markov chain with transition matrix $\boldsymbol{P}$.

Proof. For states $i, j, i_0, i_1, \dots$, consider

$$\begin{aligned}
P(X_{S+1} &= j, X_S = i, X_u = i_u, 0 \leq u < S) \\
&= \sum_s P(S = s, X_{s+1} = j, X_s = i, X_u = i_u, 0 \leq u < s) \\
&= \sum_s P(S = s | X_{s+1} = j, X_s = i, X_u = i_u, 0 \leq u < s) \\
&\quad \times P(X_{s+1} = j | X_s = i, X_u = i_u, 0 \leq u < s) \\
&\quad \times P(X_s = i, X_u = i_u, 0 \leq u < s)
\end{aligned}$$

$$= \sum_s P(S = s | X_s = i, X_u = i_u, 0 \le u < s)$$
$$\times P_{ij} P(X_s = i, X_u = i_u, 0 \le u < s)$$
$$= P_{ij} P(X_S = i, X_u = i_u, 0 \le u < S).$$

The third equality is by conditional probability. The fourth equality is because (i) S is a stopping time and the event $\{S = s\}$ is determined by $X_0, \ldots, X_s$, and (ii) by the Markov property. It follows that

$$P(X_{S+1} = j | X_S = i, X_u = i_u, 0 \le u < S)$$
$$= \frac{P(X_{S+1} = j, X_S = i, X_u = i_u, 0 \le u < S)}{P(X_S = i, X_u = i_u, 0 \le u < S)}$$
$$= P_{ij}.$$

■

3.10 PROOFS OF LIMIT THEOREMS*

In this section, we prove the main limit theorems from this chapter. Each proof is given after restating the corresponding theorem.

Limit Theorem for Regular Markov Chains

Theorem 3.2. *A Markov chain whose transition matrix* $\boldsymbol{P}$ *is regular has a limiting distribution, which is the unique, positive, stationary distribution of the chain.*

Proof of Theorem 3.2. This is a direct consequence of two forthcoming results: Proposition 3.13, which gives that regular Markov chains are ergodic, and Theorem 3.8, the fundamental limit theorem for ergodic Markov chains. ■

Finite Irreducible Markov Chains

Theorem 3.6. *Assume that* $X_0, X_1, \ldots$ *is a finite irreducible Markov chain. For each state* j, *let* $\mu_j = E(T_j | X_0 = j)$ *be the expected return time to* j. *Then,* μ_j *is finite, and there exists a unique, positive stationary distribution* $\boldsymbol{\pi}$ *such that*

$$\pi_j = \frac{1}{\mu_j}, \text{ for all } j. \tag{3.14}$$

Furthermore, for all i *and* j,

$$\pi_j = \lim_{n \to \infty} \frac{1}{n} \sum_{m=0}^{n-1} P_{ij}^m. \tag{3.15}$$

Proof of Theorem 3.6. Let $X_0, X_1, \ldots$ be an irreducible Markov chain with state space $\{1, \ldots, k\}$. Given states i, j, consider the chain started in i. Since the chain is irreducible and all states are recurrent, the chain will visit j infinitely often.

Let Y_1 be the time the chain first hits j. Since j is recurrent, the chain will return to j infinitely often. For $n \geq 2$, let Y_n be the number of steps from the $(n-1)$st visit to j to the nth visit to j. By the strong Markov property, each time the chain visits j it probabilistically restarts itself independently of past history. Thus, $Y_1, Y_2, \ldots$ is an i.i.d. sequence with common mean $\mu_j = E(T_j | X_0 = j)$.

Assume that $\mu_j < \infty$. By the strong law of large numbers,

$$\lim_{n\to\infty} \frac{Y_1 + \cdots + Y_n}{n} = \mu_j, \text{ with probability } 1. \tag{3.16}$$

Define indicator variables

$$I_m = \begin{cases} 1, & \text{if } X_m = j, \\ 0, & \text{otherwise,} \end{cases}$$

for $m = 0, 1, \ldots$ Then, $\sum_{m=0}^{n-1} I_m$ is the number of visits to j in the first n steps of the chain. The long-term expected proportion of visits to j is

$$\lim_{n\to\infty} E\left(\frac{1}{n}\sum_{m=0}^{n-1} I_m\right) = \lim_{n\to\infty} \frac{1}{n}\sum_{m=0}^{n-1} E(I_m) = \lim_{n\to\infty} \frac{1}{n}\sum_{m=0}^{n-1} P_{ij}^m.$$

Since there are n visits to j by time $Y_1 + \cdots + Y_n$, for large n,

$$\frac{1}{n}\sum_{m=0}^{n-1} I_m \approx \frac{n}{Y_1 + \cdots + Y_n},$$

giving that

$$\lim_{n\to\infty} \frac{1}{n}\sum_{m=0}^{n-1} P_{ij}^m = \lim_{n\to\infty} \frac{n}{Y_1 + \cdots + Y_n} = \frac{1}{\mu_j}, \text{with probability } 1. \tag{3.17}$$

Let $\pi_j = 1/\mu_j$, for all j. Then, $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_k)$ is the desired stationary distribution by the following four properties.

1. Since the μ_j are positive and finite, $\boldsymbol{\pi}$ is positive.
2. Summing the entries of $\boldsymbol{\pi}$ gives

$$\sum_{j=1}^{k} \pi_j = \sum_{j=1}^{k} \lim_{n\to\infty} \frac{1}{n}\sum_{m=0}^{n-1} P_{ij}^m = \lim_{n\to\infty} \frac{1}{n}\sum_{m=0}^{n-1}\sum_{j=1}^{k} P_{ij}^m = \lim_{n\to\infty} \frac{1}{n}\sum_{m=0}^{n-1} 1 = 1.$$

Thus, $\boldsymbol{\pi}$ is a probability distribution.

3. To show $\boldsymbol{\pi}$ is a stationary distribution, we need to show that

$$\sum_{i=1}^{k} \frac{1}{\mu_i} P_{ij} = \frac{1}{\mu_j}.$$

We have that

$$\begin{aligned}
\sum_{i=1}^{k} \frac{1}{\mu_i} P_{ij} &= \sum_{i=1}^{k} \left(\lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} P_{ii}^m \right) P_{ij} \\
&= \lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} \sum_{i=1}^{k} P_{ii}^m P_{ij} \\
&= \lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} P_{ij}^{m+1} \\
&= \lim_{n\to\infty} \left(\frac{n+1}{n}\right) \left(\frac{1}{n+1}\right) \left(\sum_{m=0}^{n} P_{ij}^m - P_{ij}^0 \right) \\
&= \left(\lim_{n\to\infty} \frac{n+1}{n} \right) \left(\lim_{n\to\infty} \frac{1}{n+1} \sum_{m=0}^{n} P_{ij}^m \right) - \lim_{n\to\infty} \frac{P_{ij}^0}{n+1} \\
&= \frac{1}{\mu_j}.
\end{aligned}$$

4. For uniqueness, assume that $\boldsymbol{\pi} = \boldsymbol{\pi P}$ is a stationary distribution. Then, $\boldsymbol{\pi} = \boldsymbol{\pi P}^n$, for all n, and thus $\boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\pi P}^n$. Pointwise,

$$\begin{aligned}
\pi_j &= \lim_{n\to\infty} \sum_{i=1}^{k} \pi_i P_{ij}^n = \lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} \sum_{i=1}^{k} \pi_i P_{ij}^m \\
&= \sum_{i=1}^{k} \pi_i \lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} P_{ij}^m = \sum_{i=1}^{k} \pi_i \frac{1}{\mu_j} = \frac{1}{\mu_j}.
\end{aligned}$$

For the second equality, we use the fact that if a sequence converges to a limit, then the sequence of partial averages also converges to that limit. We have shown that if $\boldsymbol{\pi}$ is a stationary distribution, then necessarily $\pi_j = 1/\mu_j$.

To finish the proof of Theorem 3.6, it remains to show that for a finite Markov chain the expected return time μ_j is finite, for all j. A recurrent state j with finite expected return time is called positive recurrent. If the expected return time is infinite, the state is called null recurrent.

To show that the states of a finite irreducible Markov chain are all positive recurrent, we show that a finite irreducible Markov chain contains at least one positive recurrent state. The result will follow as a consequence of the following lemma.

Positive and Null Recurrence are Class Properties

Lemma 3.12. *All the states in a recurrent communication class are either positive recurrent or null recurrent.*

Proof of Lemma. Assume that i is a positive recurrent state. Let j be another state in the same communication class as i. Since both states communicate, there exist positive integers r and s such that $P^r_{ji} > 0$ and $P^s_{ij} > 0$. Thus,

$$\begin{aligned}
\frac{1}{\mu_j} &= \lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} P^m_{jj} \\
&\geq \lim_{n\to\infty} \frac{1}{n} \sum_{m=r+s}^{n-1} P^r_{ji} P^{m-r-s}_{ii} P^s_{ij} \\
&= \lim_{n\to\infty} \left(\frac{n-r-s}{n}\right) P^r_{ji} \left(\frac{1}{n-r-s} \sum_{m=r+s}^{n-1} P^{m-r-s}_{ii}\right) P^s_{ij} \\
&= P^r_{ji} \left(\frac{1}{\mu_i}\right) P^s_{ij} > 0.
\end{aligned}$$

Hence, $\mu_j < \infty$ and j is positive recurrent. Having shown that positive recurrence is a class property, it follows that null recurrence is a class property. For if the communication class of a null recurrent state contains a positive recurrent state, then all states in the class are positive recurrent, leading to a contradiction. ■

A finite irreducible Markov chain is recurrent. We show that at least one state must be positive recurrent. If not, then all states are null recurrent, and all expected return times are infinite. See Equation (3.16). Since the Y_i are non-negative, this equation still holds with $\mu_j = +\infty$. And by Equation (3.17),

$$\lim_{n\to\infty} \frac{1}{n} \sum_{m=1}^{n} P^m_{ij} = 0, \text{ for all } i, j.$$

Sum over j to obtain

$$\begin{aligned}
0 &= \sum_{j=1}^{k} \lim_{n\to\infty} \frac{1}{n} \sum_{m=1}^{n} P^m_{ij} = \lim_{n\to\infty} \frac{1}{n} \sum_{j=1}^{k} \sum_{m=1}^{n} P^m_{ij} \\
&= \lim_{n\to\infty} \frac{1}{n} \sum_{m=1}^{n} \sum_{j=1}^{k} P^m_{ij} = \lim_{n\to\infty} \frac{1}{n} \sum_{m=1}^{n} 1 = 1,
\end{aligned}$$

a contradiction. Thus, a finite irreducible Markov chain contains at least one positive recurrent state. By Lemma 3.12, all states are positive recurrent. And Theorem 3.6 is proved. ■

Remark: The theorem holds for infinite irreducible chains that are positive recurrent. For infinite irreducible chains that are null recurrent, no stationary distribution exists.

Fundamental Limit Theorem for Ergodic Markov Chains

Theorem 3.8. *Let $X_0, X_1, \ldots$ be an ergodic Markov chain. There exists a unique, positive, stationary distribution $\boldsymbol{\pi}$, which is the limiting distribution of the chain. That is,*

$$\pi_j = \lim_{n\to\infty} P^n_{ij}, \text{ for all } i, j.$$

Proof of Theorem 3.8. Two proofs will be given. One is probabilistic, based on an elegant technique known as *coupling*. The other relies on linear algebra and the eigenstructure of the transition matrix.

Both proofs are a consequence of the following proposition, which says that finite ergodic Markov chains are precisely those chains that have regular transition matrices. Recall that a square matrix is regular if some power of the matrix has all positive entries.

Ergodic Chains and Regular Matrices

Proposition 3.13. *Assume that $\boldsymbol{P}$ is the transition matrix of a finite Markov chain. The Markov chain is ergodic if and only if $\boldsymbol{P}$ is regular.*

The proof of this proposition relies on the following lemma.

Lemma 3.14. *If i is an aperiodic state, there exists a positive integer N such that $P^n_{ii} > 0$ for all $n \geq N$.*

Proof of Lemma. The following is based on Hoel et al. (1986) and uses results from number theory.

Assume that i is an aperiodic state. Let $T = \{n > 0 : P^n_{ii} > 0\}$. By definition, $\gcd(T) = 1$. The set T is closed under addition, since if $m, n \in T$, then

$$P^{m+n}_{ii} = \sum_k P^m_{ik} P^n_{ki} \geq P^m_{ii} P^m_{ii} > 0.$$

That is, $m + n \in T$.

We claim that T contains two consecutive integers. If not, then there exists $k, m \in T$ such that $k \geq 2$, $k + m \in T$, and any two integers in T differ by at least k. Furthermore, since $\gcd(T) = 1$, there is an $n \in T$ such that k is not a divisor of n. Write $n = qk + r$, where $q \geq 0$ and $0 < r < k$. Since T is closed under addition, $(q + 1)(m + k) \in T$ and $n + (q + 1)m \in T$. Their difference is

$$(q + 1)(m + k) - n - (q + 1)m = k + qk - n = k - r > 0.$$

Thus, we have found two elements of T whose difference is positive and smaller than k, giving a contradiction.

Hence, T contains consecutive integers, say m and $m+1$. Let $N = m^2$. We show that $n \in T$, for all $n \geq N$, which establishes the lemma. For $n \geq N$, write $n - N = qm + r$, for $q \geq 0$ and $0 \leq r < m$. Then,

$$n = m^2 + qm + r = (m - r + q)m + r(m+1) \in T. \qquad \blacksquare$$

Proof of Proposition 3.13. Assume that $\boldsymbol{P}$ is the transition matrix of a finite ergodic chain. Since the chain is irreducible, for states i and j there exists $m \geq 0$, such that $P^m_{ij} > 0$. The number $m = m(i,j)$ depends on i and j. Let $M^* = \max_{i,j} m(i,j)$. We can take the maximum since the chain is finite.

Since the chain is aperiodic, by Lemma 3.14, there exists $N > 0$ such that $P^n_{ii} > 0$, for all $n \geq N$. The number $N = N(i)$ depends on i. Let $N^* = \max_i N(i)$. Then, N^* does not depend on i, and for all $n \geq N^*$, $P^n_{ii} > 0$, for all i.

Let $X = M^* + N^*$. We claim that $\boldsymbol{P}^X$ is positive. For states i and j,

$$P^X_{ij} = P^{(X-m(i,j))+m(i,j)}_{ij} = \sum_{t=1}^{k} P^{X-m(i,j)}_{it} P^{m(i,j)}_{tj} \geq P^{X-m(i,j)}_{ii} P^{m(i,j)}_{ij} > 0.$$

The last inequality is because (i) $P^{m(i,j)}_{ij} > 0$, and (ii) $P^{X-m(i,j)}_{ii} > 0$, since

$$X - m(i,j) \geq X - M^* = N^*.$$

Thus, $\boldsymbol{P}$ is regular.

Conversely, assume that $\boldsymbol{P}$ is regular. Then, $\boldsymbol{P}^n > 0$ for some positive integer N. Thus, all states communicate and the chain is irreducible. It suffices to show that the chain is aperiodic. Stochastic matrices have the property that if $\boldsymbol{P}^n$ is positive then $\boldsymbol{P}^{N+m}$ is positive for all $m \geq 0$, a property we leave for the reader to prove. (See Exercise 3.33.) For any state i, the set of possible return times to i includes $N, N+1, \ldots$, and gcd $\{N, N+1, \ldots\} = 1$. That is, i is aperiodic. $\blacksquare$

Coupling Proof of Fundamental Limit Theorem

The method of proof is based on *coupling*, a probabilistic technique first introduced by the German mathematician Wolfgang Doeblin in the 1930s.

Here is a bird's-eye view. Let $X_0, X_1, \ldots$ be an ergodic Markov chain on $\mathcal{S}$ with transition matrix $\boldsymbol{P}$. Since the chain is irreducible, it has a unique stationary distribution $\boldsymbol{\pi}$. We need to show that for all i and j,

$$\lim_{n\to\infty} P(X_n = j | X_0 = i) = \pi_j.$$

Consider a second chain $Y_0, Y_1, \ldots$ with the same transition matrix $\boldsymbol{P}$, but with initial distribution $\boldsymbol{\pi}$. That is, the Y chain is a stationary chain. For all $n \geq 0$, the distribution of Y_n is $\boldsymbol{\pi}$.

The X and Y chains are run independently of each other. Eventually, at some finite time T, both chains will hit the same state. The chains are then *coupled* so that $X_n = Y_n$, for $n \geq T$. Since the Y chain is in stationarity, from time T onwards the X chain is also in stationarity, from which follows the result.

To elaborate, let $T = \min\{n \geq 0 : X_n = Y_n\}$ be the first time that the X and Y chains hit the same state. Define a new process by letting

$$Z_n = \begin{cases} X_n, & \text{if } n < T, \\ Y_n, & \text{if } n \geq T, \end{cases}$$

for $n \geq 0$. Then, $Z_0, Z_1, \ldots$ is a Markov chain with the same transition matrix and initial distribution as the X chain.

Consider the bivariate process $(Z_0, Y_0), (Z_1, Y_1), \ldots$ The bivariate process is a Markov chain on the state space $\mathcal{S} \times \mathcal{S}$ with transition matrix $\widetilde{\boldsymbol{P}}$ defined by

$$\widetilde{P}_{(i,k),(j,l)} = P_{ij}P_{kl}.$$

The bivariate process represents a *coupling* of the original X chain with the stationary Y chain. The chains are coupled in such a way so that once both chains hit the same state then from that time onward the chains march forward in lockstep. See Example 3.34 for an illustration of the construction.

We show that the bivariate Markov chain is ergodic. Since the X chain is ergodic, $\boldsymbol{P}$ is regular, and there exists some $N > 0$ such that $\boldsymbol{P}^N > 0$. For this choice of N, and for all i, j, k, l,

$$\widetilde{P}^N_{(i,k),(j,l)} = P^N_{ij}P^N_{kl} > 0.$$

Thus, $\widetilde{\boldsymbol{P}}$ is regular, and by Proposition 3.13 the bivariate chain is ergodic. From any state, the bivariate chain reaches any other state in finite time, with probability 1. In particular, it eventually hits a state of the form (j, j). The event that $(Z_n, Y_n) = (j, j)$ for some j implies that the two chains have coupled by time n. It follows that T, the first time the two chains meet, is finite with probability 1. Hence,

$$\lim_{n\to\infty} P(T > n) = \lim_{n\to\infty} 1 - P(T \leq n) = 1 - P(T < \infty) = 0.$$

Consider

$$P(Y_n = j) = P(Y_n = j, T \leq n) + P(Y_n = j, T > n).$$

Taking limits, as $n \to \infty$, the left-hand side converges to π_j, and the rightmost term converges to 0. Thus, $P(Y_n = j, T \leq n) \to \pi_j$, as $n \to \infty$.

For any initial distribution,

$$\begin{aligned} P(X_n = j) &= P(Z_n = j) \\ &= P(Z_n = j, T \leq n) + P(Z_n = j, T > n) \\ &= P(Z_n = j | T \leq n)P(T \leq n) + P(Z_n = j, T > n) \\ &= P(Y_n = j | T \leq n)P(T \leq n) + P(Z_n = j, T > n) \\ &= P(Y_n = j, T \leq n) + P(Z_n = j, T > n). \end{aligned}$$

Taking limits gives

$$\lim_{n\to\infty} P(X_n = j) = \lim_{n\to\infty} P(Y_n = j, T \le n) + \lim_{n\to\infty} P(Z_n = j, T > n) = \pi_j,$$

which completes the proof. ■

Example 3.34 The coupling construction is illustrated on a two-state chain with state space $\mathcal{S} = \{a, b\}$ and transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ a \\ b \end{array}\!\!\begin{array}{c} \begin{array}{cc} a & \quad b \end{array} \\ \begin{pmatrix} 9/10 & 1/10 \\ 1/5 & 4/5 \end{pmatrix} \end{array}.$$

The chain is ergodic with stationary distribution $\boldsymbol{\pi} = (2/3, 1/3)$.

For the following simulation, the X chain was started at a, the Y chain in $\boldsymbol{\pi}$. Both chains were run independently for 12 steps. The chains coupled at time $T = 8$.

Chain	0	1	2	3	4	5	6	7	8	9	10	11	12
X	a	a	a	a	a	b	b	b	a	a	b	a	a
Y	b	b	b	b	b	a	a	a	a	a	b	b	b
Z	a	a	a	a	a	b	b	b	a	a	b	b	b
(Z, Y)	ab	ab	ab	ab	ab	ba	ba	ba	aa	aa	bb	bb	bb

The transition matrix $\widetilde{\boldsymbol{P}}$ of the bivariate process is

$$\widetilde{\boldsymbol{P}} = \begin{array}{c} \\ aa \\ ab \\ ba \\ bb \end{array}\!\!\begin{array}{c} \begin{array}{cccc} aa & ab & ba & bb \end{array} \\ \begin{pmatrix} (9/10)^2 & (9/10)(1/10) & (1/10)(9/10) & (1/10)^2 \\ (9/10)(1/5) & (9/10)(4/5) & (1/10)(1/5) & (1/10)(4/5) \\ (1/5)(9/10) & (1/5)(1/10) & (4/5)(9/10) & (4/5)(1/10) \\ (1/5)^2 & (1/5)(4/5) & (4/5)(1/5) & (4/5)^2 \end{pmatrix} \end{array}$$

$$= \begin{array}{c} \\ aa \\ ab \\ ba \\ bb \end{array}\!\!\begin{array}{c} \begin{array}{cccc} aa & ab & ba & bb \end{array} \\ \begin{pmatrix} 81/100 & 9/100 & 9/100 & 1/100 \\ 9/50 & 36/50 & 1/50 & 4/50 \\ 9/50 & 1/50 & 36/50 & 4/50 \\ 1/25 & 4/25 & 4/25 & 16/25 \end{pmatrix} \end{array}.$$

■

Linear Algebra Proof of Fundamental Limit Theorem

Asymptotic properties of Markov chains are related to the eigenstructure of the transition matrix.

Eigenvalues of a Stochastic Matrix

Lemma 3.15. *A stochastic matrix* $\boldsymbol{P}$ *has an eigenvalue* $\lambda^* = 1$. *All other eigenvalues* λ *of* $\boldsymbol{P}$ *are such that* $|\lambda| \leq 1$.

If $\boldsymbol{P}$ *is a regular matrix, then the inequality is strict. That is,* $|\lambda| < 1$ *for all* $\lambda \neq \lambda^*$.

Proof. Let $\boldsymbol{P}$ be a $k \times k$ stochastic matrix. Since the rows of $\boldsymbol{P}$ sum to 1, we have that $\boldsymbol{P1} = \boldsymbol{1}$, where $\boldsymbol{1}$ is a column vector of all 1s. Thus, $\lambda^* = 1$ is an eigenvalue of $\boldsymbol{P}$. Let λ be any other eigenvalue of $\boldsymbol{P}$ with corresponding eigenvector $\boldsymbol{z}$. Let $|z_m| = \max_{1 \leq i \leq k} |z_i|$. That is, z_m is the component of $\boldsymbol{z}$ of maximum absolute value. Then,

$$|\lambda||z_m| = |\lambda z_m| = |(Pz)_m| = \left| \sum_{i=1}^{k} P_{mi} z_i \right| \leq \sum_{i=1}^{k} P_{mi} |z_i| \leq |z_m| \sum_{i=1}^{k} P_{mi} = |z_m|.$$

Thus, $|\lambda| \leq 1$.

Assume that $\boldsymbol{P}$ is regular. Then, $\boldsymbol{P}^N > 0$, for some $N > 0$. Since $\boldsymbol{P}^N$ is a stochastic matrix, the first part of the lemma holds for $\boldsymbol{P}^N$. If λ is an eigenvalue of $\boldsymbol{P}$, then λ^N is an eigenvalue of $\boldsymbol{P}^N$. Let $\boldsymbol{x}$ be the corresponding eigenvector, with $|x_m| = \max_{1 \leq i \leq k} |x_i|$. Then,

$$|\lambda|^N |x_m| = |(P^N x)_m| = \left| \sum_{i=1}^{k} P^N_{mi} x_i \right| \leq \sum_{i=1}^{k} P^N_{mi} |x_i| \leq |x_m| \sum_{i=1}^{k} P^N_{mi} = |x_m|.$$

Since the entries of $\boldsymbol{P}^N$ are all positive, the last inequality is an equality only if $|x_1| = |x_2| = \cdots = |x_k|$. And the first inequality is an equality only if $x_1 = \cdots = x_k$. But the constant vector whose components are all the same is an eigenvector associated with the eigenvalue 1. Hence, if $\lambda \neq 1$, one of the inequalities is strict. Thus, $|\lambda|^N < 1$, and the result follows. ∎

The fundamental limit theorem for ergodic Markov chains is a consequence of the Perron–Frobenius theorem for positive matrices.

Perron–Frobenius Theorem

Theorem 3.16. *Let* $\boldsymbol{M}$ *be a* $k \times k$ *positive matrix. Then, the following statements hold.*

1. *There is a positive real number* λ^* *which is an eigenvalue of* $\boldsymbol{M}$. *For all other eigenvalues* λ *of* $\boldsymbol{M}$, $|\lambda| < \lambda^*$. *The eigenvalue* λ^* *is called the Perron–Frobenius eigenvalue.*
2. *The eigenspace of eigenvectors associated with* λ^* *is one-dimensional.*

3. *There exists a positive right eigenvector* $\boldsymbol{v}$ *associated with* λ^**, and a positive left eigenvector* $\boldsymbol{w}$ *associated with* λ^**. Furthermore,*

$$\lim_{n\to\infty} \frac{1}{(\lambda^*)^n}\boldsymbol{M}^n = \boldsymbol{v}\boldsymbol{w}^T,$$

where the eigenvectors are normalized so that $\boldsymbol{w}^T\boldsymbol{v} = 1$.

The proof of the Perron–Frobenius theorem can be found in many advanced linear algebra textbooks, including Horn and Johnson (1990).

For an ergodic Markov chain, the transition matrix $\boldsymbol{P}$ is regular and $\boldsymbol{P}^N$ is a positive matrix for some integer N. The Perron–Frobenius theorem applies. The Perron–Frobenius eigenvalue of $\boldsymbol{P}^n$ is $\lambda^* = 1$, with associated right eigenvector $\boldsymbol{v} = \mathbf{1}$, and associated left eigenvector $\boldsymbol{w}$.

If $\lambda^* = 1$ is an eigenvalue of $\boldsymbol{P}^N$, then $(\lambda^*)^{1/N} = 1$ is an eigenvalue of $\boldsymbol{P}$, with associated right and left eigenvectors $\boldsymbol{v}$ and $\boldsymbol{w}$, respectively. Normalizing $\boldsymbol{w}$ so that its components sum to 1 gives the unique, positive stationary distribution $\boldsymbol{\pi}$, which is the limiting distribution of the chain. The limiting matrix $\boldsymbol{v}\boldsymbol{w}^T$ is a stochastic matrix all of whose rows are equal to $\boldsymbol{w}^T$. ■

EXERCISES

3.1 Consider a Markov chain with transition matrix

$$\boldsymbol{P} = \begin{pmatrix} 1/2 & 1/4 & 0 & 1/4 \\ 0 & 1/2 & 1/2 & 0 \\ 1/4 & 1/4 & 1/2 & 0 \\ 0 & 1/4 & 1/2 & 1/4 \end{pmatrix}.$$

Find the stationary distribution. Do not use technology.

3.2 A stochastic matrix is called *doubly stochastic* if its rows and columns sum to 1. Show that a Markov chain whose transition matrix is doubly stochastic has a stationary distribution, which is uniform on the state space.

3.3 Determine which of the following matrices are regular.

$$\boldsymbol{P} = \begin{pmatrix} 0.4 & 0.6 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{Q} = \begin{pmatrix} 0 & 1 \\ p & 1-p \end{pmatrix}, \quad \boldsymbol{R} = \begin{pmatrix} 0 & 1 & 0 \\ 0.25 & 0.5 & 0.25 \\ 1 & 0 & 0 \end{pmatrix}.$$

3.4 Consider a Markov chain with transition matrix

$$\boldsymbol{P} = \begin{pmatrix} 1-a & a & 0 \\ 0 & 1-b & b \\ c & 0 & 1-c \end{pmatrix},$$

where $0 < a, b, c < 1$. Find the stationary distribution.

3.5 A Markov chain has transition matrix

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1/4 & 0 & 0 & 3/4 \\ 3/4 & 0 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1/4 & 3/4 & 0 & 0 & 0 \end{pmatrix}.$$

(a) Describe the set of stationary distributions for the chain.

(b) Use technology to find $\lim_{n\to\infty}\boldsymbol{P}^n$. Explain the long-term behavior of the chain.

(c) Explain why the chain does not have a limiting distribution, and why this does not contradict the existence of a limiting matrix as shown in (b).

3.6 Consider a Markov chain with transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & \cdots \end{array} \\ \begin{pmatrix} 1/2 & 1/2 & 0 & 0 & 0 & \cdots \\ 2/3 & 0 & 1/3 & 0 & 0 & \cdots \\ 3/4 & 0 & 0 & 1/4 & 0 & \cdots \\ 4/5 & 0 & 0 & 0 & 1/5 & \cdots \\ 5/6 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{array},$$

defined by

$$P_{ij} = \begin{cases} i/(i+1), & \text{if } j = 1, \\ 1/(i+1), & \text{if } j = i+1, \\ 0, & \text{otherwise.} \end{cases}$$

(a) Does the chain have a stationary distribution? If yes, exhibit the distribution. If no, explain why.

(b) Classify the states of the chain.

(c) Repeat part (a) with the row entries of $\boldsymbol{P}$ switched. That is, let

$$P_{ij} = \begin{cases} 1/(i+1), & \text{if } j = 1, \\ i/(i+1), & \text{if } j = i+1, \\ 0, & \text{otherwise.} \end{cases}$$

3.7 A Markov chain has n states. If the chain is at state k, a coin is flipped, whose heads probability is p. If the coin lands heads, the chain stays at k. If the coin lands tails, the chain moves to a different state uniformly at random. Exhibit the transition matrix and find the stationary distribution.

3.8 Let

$$\boldsymbol{P}_1 = \begin{pmatrix} 1/4 & 3/4 \\ 1/2 & 1/2 \end{pmatrix} \quad \text{and} \quad \boldsymbol{P}_2 = \begin{pmatrix} 1/5 & 4/5 \\ 4/5 & 1/5 \end{pmatrix}.$$

Consider a Markov chain on four states whose transition matrix is given by the block matrix

$$\boldsymbol{P} = \begin{pmatrix} \boldsymbol{P}_1 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{P}_2 \end{pmatrix}.$$

(a) Does the Markov chain have a unique stationary distribution? If so, find it.

(b) Does $\lim_{n\to\infty} \boldsymbol{P}^n$ exist? If so, find it.

(c) Does the Markov chain have a limiting distribution? If so, find it.

3.9 Let $\boldsymbol{P}$ be a stochastic matrix.

(a) If $\boldsymbol{P}$ is regular, is $\boldsymbol{P}^2$ regular?

(b) If $\boldsymbol{P}$ is the transition matrix of an irreducible Markov chain, is $\boldsymbol{P}^2$ the transition matrix of an irreducible Markov chain?

3.10 A Markov chain has transition matrix $\boldsymbol{P}$ and limiting distribution $\boldsymbol{\pi}$. Further assume that $\boldsymbol{\pi}$ is the initial distribution of the chain. That is, the chain is in stationarity. Find the following:

(a) $\lim_{n\to\infty} P(X_n = j|X_{n-1} = i)$

(b) $\lim_{n\to\infty} P(X_n = j|X_0 = i)$

(c) $\lim_{n\to\infty} P(X_{n+1} = k, X_n = j|X_0 = i)$

(d) $\lim_{n\to\infty} P(X_0 = j|X_n = i)$

3.11 Consider a simple symmetric random walk on $\{0, 1, \ldots, k\}$ with reflecting boundaries. If the walk is at state 0, it moves to 1 on the next step. If the walk is at k, it moves to $k - 1$ on the next step. Otherwise, the walk moves left or right, with probability 1/2.

(a) Find the stationary distribution.

(b) For $k = 1,000$, if the walk starts at 0, how many steps will it take, on average, for the walk to return to 0?

3.12 A Markov chain has transition matrix

$$\boldsymbol{P} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1/4 & 0 & 3/4 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & 3/4 & 0 & 1/4 \end{pmatrix}.$$

Find the set of all stationary distributions.

3.13 Find the communication classes of a Markov chain with transition matrix

$$P = \begin{array}{c c} & \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} & \begin{pmatrix} 1/2 & 0 & 0 & 0 & 1/2 \\ 1/3 & 1/2 & 1/6 & 0 & 0 \\ 0 & 1/4 & 0 & 1/2 & 1/4 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} \end{array}.$$

Rewrite the transition matrix in canonical form.

3.14 The California Air Resources Board warns the public when smog levels are above certain thresholds. Days when the board issues warnings are called *episode* days. Lin (1981) models the daily sequence of episode and nonepisode days as a Markov chain with transition matrix

$$P = \begin{array}{c c} & \begin{array}{cc} \text{Nonepisode} & \text{Episode} \end{array} \\ \begin{array}{c} \text{Nonepisode} \\ \text{Episode} \end{array} & \begin{pmatrix} 0.77 & 0.23 \\ 0.24 & 0.76 \end{pmatrix} \end{array}.$$

(a) What is the long-term probability that a given day will be an episode day?

(b) Over a year's time about how many days are expected to be episode days?

(c) In the long-term, what is the average number of days that will transpire between episode days?

3.15 On a chessboard a single random knight performs a simple random walk. From any square, the knight chooses from among its permissible moves with equal probability. If the knight starts on a corner, how long, on average, will it take to return to that corner?

3.16 As in the previous exercise, find the expected return time from a corner square for the following chess pieces: (i) queen, (ii) rook, (iii) king, (iv) bishop. Order the pieces by which pieces return quickest.

3.17 Consider a Markov chain with transition matrix

$$P = \begin{pmatrix} 1/2 & 1/2 \\ 0 & 1 \end{pmatrix}.$$

Obtain a closed form expression for P^n. Exhibit the matrix $\sum_{n=0}^{\infty} P^n$ (some entries may be $+\infty$). Explain what this shows about the recurrence and transience of the states.

3.18 Use first-step analysis to find the expected return time to state b for the Markov chain with transition matrix

$$\begin{array}{cc} & \begin{array}{ccc} a & b & c \end{array} \\ \boldsymbol{P} = \begin{array}{c} a \\ b \\ c \end{array} & \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/4 & 0 & 3/4 \\ 1/2 & 1/2 & 0 \end{pmatrix} \end{array}.$$

3.19 Consider random walk on the graph in Figure 3.15. Use first-step analysis to find the expected time to hit d for the walk started in a. (*Hint*: By exploiting symmetries in the graph, the solution can be found by solving a 3×3 linear system.)

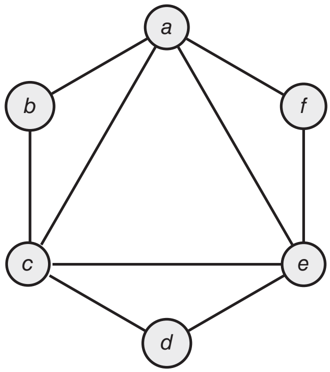

Figure 3.15

3.20 Show that simple symmetric random walk on $\mathbb{Z}^2$, that is, on the integer points in the plane, is recurrent. As in the one-dimensional case, consider the origin.

3.21 Show that simple symmetric random walk on $\mathbb{Z}^3$ is transient. As in the one-dimensional case, consider the origin and show

$$\begin{aligned} P_{00}^{2n} &= \frac{1}{6^{2n}} \sum_{0 \le j+k \le n} \frac{(2n)!}{j!j!k!k!(n-j-k)!(n-j-k)!}, \\ &\le \frac{1}{2^{2n}} \binom{2n}{n} \left(\frac{1}{3^n} \frac{n!}{(n/3)!(n/3)!(n/3)!} \right). \end{aligned}$$

Then, use Stirling's approximation.

3.22 Consider the general two-state chain

$$\begin{array}{cc} & \begin{array}{cc} 1 & 2 \end{array} \\ \boldsymbol{P} = \begin{array}{c} 1 \\ 2 \end{array} & \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix} \end{array},$$

where p and q are not both 0. Let T be the first return time to state 1, for the chain started in 1.

(a) Show that $P(T \geq n) = p(1-q)^{n-2}$, for $\quad n \geq 2$.

(b) Find $E(T)$ and verify that $E(T) = 1/\pi_1$, where $\boldsymbol{\pi}$ is the stationary distribution of the chain.

3.23 Consider a k-state Markov chain with transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ \vdots \\ k-2 \\ k-1 \\ k \end{array} \begin{array}{c} \begin{array}{ccccccc} 1 & 2 & 3 & \cdots & k-2 & k-1 & k \end{array} \\ \begin{pmatrix} 1/k & 1/k & 1/k & \cdots & 1/k & 1/k & 1/k \\ 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix} \end{array}.$$

Show that the chain is ergodic and find the limiting distribution.

3.24 Show that the stationary distribution for the modified Ehrenfest chain of Example 3.19 is binomial with parameters N and 1/2.

3.25 Read about the Bernoulli–Laplace model of diffusion in Exercise 2.12.

(a) Find the stationary distribution for the cases $k = 2$ and $k = 3$.

(b) For general k, show that $\pi_j = \binom{k}{j}^2 / \binom{2k}{k}$, for $j = 0, 1, \ldots, k$, satisfies the equations for the stationary distribution and is thus the unique limiting distribution of the chain.

3.26 Assume that $(p_1, \ldots, p_k)$ is a probability vector. Let $\boldsymbol{P}$ be a $k \times k$ transition matrix defined by

$$P_{ij} = \begin{cases} p_j, & \text{if } i = 1, \ldots, k-1, \\ 0, & \text{if } i = k, j < k, \\ 1, & \text{if } i = k, j = k. \end{cases}$$

Describe all the stationary distributions for $\boldsymbol{P}$.

3.27 Sinclair (2005). Consider the infinite Markov chain on the non-negative integers described by Figure 3.16.

(a) Show that the chain is irreducible and aperiodic.

(b) Show that the chain is recurrent by computing the first return time to 0 for the chain started at 0.

(c) Show that the chain is null recurrent.

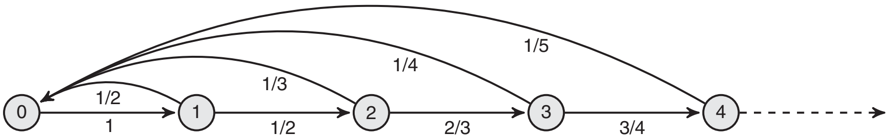

Figure 3.16

3.28 Consider a Markov chain with transition matrix

$$P = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{array} \begin{array}{c} \begin{array}{ccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{array} \\ \begin{pmatrix} 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 \\ 2/3 & 0 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 2/3 & 1/3 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 1/2 & 0 & 1/4 & 0 \\ 0 & 0 & 1/4 & 0 & 1/4 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1/8 & 1/8 & 1/8 & 1/8 & 1/4 & 1/4 \end{pmatrix} \end{array}.$$

Identify the communication classes. Classify the states as recurrent or transient. For all i and j, determine $\lim_{n\to\infty} P^n_{ij}$ without using technology.

3.29 Consider a Markov chain with transition matrix

$$P = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \\ f \\ g \end{array} \begin{array}{c} \begin{array}{ccccccc} a & b & c & d & e & f & g \end{array} \\ \begin{pmatrix} 0.6 & 0.2 & 0 & 0 & 0.2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5 & 0.5 \\ 0 & 0 & 0.3 & 0.7 & 0 & 0 & 0 \\ 0 & 0.3 & 0.4 & 0.3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0.1 & 0 & 0 & 0 & 0 & 0.9 \\ 0 & 0.2 & 0 & 0 & 0 & 0.8 & 0 \end{pmatrix} \end{array}.$$

Identify the communication classes. Classify the states as recurrent or transient, and determine the period of each state.

3.30 A graph is *bipartite* if the vertex set can be colored with two colors black and white such that every edge in the graph joins a black vertex and a white vertex. See Figure 3.7(a) for an example of a bipartite graph. Show that for simple random walk on a connected graph, the walk is periodic if and only if the graph is bipartite.

3.31 For the network graph in Figure 3.17, find the PageRank for the nodes of the network using a damping factor of $p = 0.90$. See Example 3.21.

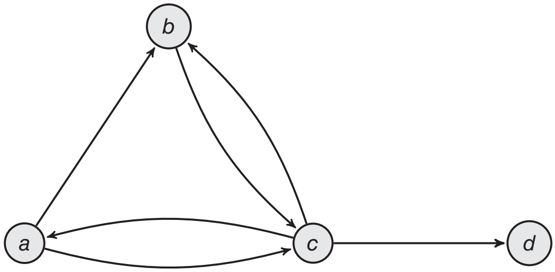

Figure 3.17

3.32 Let $X_0, X_1, \ldots$ be an ergodic Markov chain with transition matrix $\boldsymbol{P}$ and stationary distribution $\boldsymbol{\pi}$. Define the bivariate process $Z_n = (X_n, X_{n-1})$, for $n \geq 1$, with $Z_0 = (X_0, X_0)$.

(a) Give an intuitive explanation for why $Z_0, Z_1, \ldots$ is a Markov chain.

(b) Determine the transition probabilities in terms of $\boldsymbol{P}$. That is, find

$$P(Z_n = (i,j) | Z_{n-1} = (s,t)).$$

(c) Find the limiting distribution.

3.33 Assume that $\boldsymbol{P}$ is a stochastic matrix. Show that if $\boldsymbol{P}^N$ is positive, then $\boldsymbol{P}^{N+m}$ is positive for all $m \geq 0$.

3.34 Let $\boldsymbol{P}$ be the transition matrix of an irreducible, but not necessarily ergodic, Markov chain. For $0 < p < 1$, let

$$\widetilde{\boldsymbol{P}} = p\boldsymbol{P} + (1-p)\boldsymbol{I},$$

where $\boldsymbol{I}$ is the identity matrix. Show that $\widetilde{\boldsymbol{P}}$ is a stochastic matrix for an ergodic Markov chain with the same stationary distribution as $\boldsymbol{P}$. Give an intuitive description for how the $\widetilde{\boldsymbol{P}}$ chain evolves compared to the $\boldsymbol{P}$-chain.

3.35 Let $\boldsymbol{Q}$ be a $k \times k$ stochastic matrix. Let $\boldsymbol{A}$ be a $k \times k$ matrix each of whose entries is $1/k$. For $0 < p < 1$, let

$$\boldsymbol{P} = p\boldsymbol{Q} + (1-p)\boldsymbol{A}.$$

Show that $\boldsymbol{P}$ is the transition matrix for an ergodic Markov chain.

3.36 Let $X_0, X_1, \ldots$ be an ergodic Markov chain on $\{1, \ldots, k\}$ with stationary distribution $\boldsymbol{\pi}$. Assume that the chain is in stationarity.

(a) Find $\text{Cov}(X_m, X_{m+n})$.

(b) Find $\lim_{n\to\infty} \text{Cov}(X_m, X_{m+n})$.

3.37 Show that all two-state Markov chains, except for the trivial chain whose transition matrix is the identity matrix, are time reversible.

3.38 You throw five dice and set aside those dice that are sixes. Throw the remaining dice and again set aside the sixes. Continue until you get all sixes.

(a) Exhibit the transition matrix for the associated Markov chain, where X_n is the number of sixes after n throws. See also Exercise 2.11.

(b) How many turns does it take, on average, before you get all sixes?

3.39 Show that if $X_0, X_1, \ldots$ is reversible, then for the chain in stationarity

$$P(X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n) = P(X_n = i_0, X_{n-1} = i_1, \ldots, X_0 = i_n),$$

for all $i_0, i_1, \ldots, i_n$.

3.40 Consider a *biased random walk* on the n-cycle, which moves one direction with probability p and the other direction with probability $1 - p$. Determine whether the walk is time reversible.

3.41 Show that the Markov chain with transition matrix

$$\boldsymbol{P} = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{pmatrix} 1/6 & 1/6 & 0 & 2/3 \\ 1/5 & 2/5 & 2/5 & 0 \\ 0 & 1/3 & 1/6 & 1/2 \\ 4/9 & 0 & 1/3 & 2/9 \end{pmatrix} \end{array}$$

is reversible. The chain can be described by a random walk on a weighted graph. Exhibit the graph such that all the weights are integers.

3.42 Consider random walk on $\{0, 1, 2, \ldots\}$ with one reflecting boundary. If the walk is at 0, it moves to 1 on the next step. Otherwise, it moves left, with probability p, or right, with probability $1 - p$. For what values of p is the chain reversible? For such p, find the stationary distribution.

3.43 A Markov chain has transition matrix

$$\boldsymbol{P} = \begin{pmatrix} 1/2 & 1/4 & 0 & 1/4 \\ p & 0 & 1-p & 0 \\ 0 & 1/4 & 1/2 & 1/4 \\ q & 0 & 1-q & 0 \end{pmatrix}.$$

(a) For what values of p and q is the chain ergodic?

(b) For what values of p and q is the chain reversible?

3.44 Markov chains are used to model nucleotide substitutions and mutations in DNA sequences. Kimura gives the following transition matrix for such a model.

$$\boldsymbol{P} = \begin{array}{c} \\ a \\ g \\ c \\ t \end{array} \begin{array}{c} \begin{array}{cccc} a & g & c & t \end{array} \\ \begin{pmatrix} 1-p-2r & p & r & r \\ p & 1-p-2r & r & r \\ q & q & 1-p-2q & p \\ q & q & p & 1-p-2q \end{pmatrix} \end{array}.$$

Find a vector $\boldsymbol{x}$ that satisfies the detailed-balance equations. Show that the chain is reversible and find the stationary distribution. Confirm your result for the case $p = 0.1$, $q = 0.2$, and $r = 0.3$.

3.45 If $\boldsymbol{P}$ is the transition matrix of a reversible Markov chain, show that $\boldsymbol{P}^2$ is, too. Conclude that $\boldsymbol{P}^n$ is the transition matrix of a reversible Markov chain for all $n \geq 1$.

3.46 Given a Markov chain with transition matrix $\boldsymbol{P}$ and stationary distribution $\boldsymbol{\pi}$, the *time reversal* is a Markov chain with transition matrix $\widetilde{\boldsymbol{P}}$ defined by

$$\widetilde{P}_{ij} = \frac{\pi_j P_{ji}}{\pi_i}, \quad \text{for all } i,j.$$

(a) Show that a Markov chain with transition matrix $\boldsymbol{P}$ is reversible if and only if $\boldsymbol{P} = \widetilde{\boldsymbol{P}}$.

(b) Show that the time reversal Markov chain has the same stationary distribution as the original chain.

3.47 Consider a Markov chain with transition matrix

$$\boldsymbol{P} = \begin{array}{c c} & \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \end{array} & \begin{pmatrix} 1/3 & 0 & 2/3 \\ 1/2 & 1/2 & 0 \\ 1/6 & 1/3 & 1/2 \end{pmatrix} \end{array}.$$

Find the transition matrix of the time reversal chain (see Exercise 3.46).

3.48 Consider a Markov chain with transition matrix

$$\boldsymbol{P} = \begin{array}{c c} & \begin{array}{ccc} a & b & c \end{array} \\ \begin{array}{c} a \\ b \\ c \end{array} & \begin{pmatrix} 1-\alpha & \alpha & 0 \\ 0 & 1-\beta & \beta \\ \gamma & 0 & 1-\gamma \end{pmatrix} \end{array},$$

where $0 < \alpha, \beta, \gamma < 1$. Find the transition matrix of the time reversal chain (see Exercise 3.46).

3.49 Consider an absorbing chain with t transient and $k - t$ absorbing states. For transient state i and absorbing state j, let B_{ij} denote the probability starting at i that the chain is absorbed in j. Let $\boldsymbol{B}$ be the resulting $t \times (k - t)$ matrix. By first-step analysis show that $\boldsymbol{B} = (\boldsymbol{I} - \boldsymbol{Q})^{-1}\boldsymbol{R}$.

3.50 Consider the following method for shuffling a deck of cards. Pick two cards from the deck uniformly at random and then switch their positions. If the same two cards are chosen, the deck does not change. This is called the *random transpositions* shuffle.

(a) Argue that the chain is ergodic and the stationary distribution is uniform.

(b) Exhibit the 6×6 transition matrix for a three-card deck.

(c) How many shuffles does it take on average to reverse the original order of the deck of cards?

3.51 A deck of k cards is shuffled by the *top-to-random* method: the top card is placed in a uniformly random position in the deck. (After one shuffle, the top card stays where it is with probability $1/k$.) Assume that the top card of the deck is the ace of hearts. Consider a Markov chain where X_n is the position of the ace of hearts after n top-to-random shuffles, with $X_0 = 1$. The state space is $\{1, \dots, k\}$. Assume that $k = 6$.

(a) Exhibit the transition matrix and find the expected number of shuffles for the ace of hearts to return to the top of the deck.

(b) Find the expected number of shuffles for the bottom card to reach the top of the deck.

3.52 The board for a modified Snakes and Ladder game is shown in Figure 3.18. The game is played with a tetrahedron (four-faced) die.

(a) Find the expected length of the game.

(b) Assume that the player is on square 6. Find the probability that they will find themselves on square 3 before finishing the game.

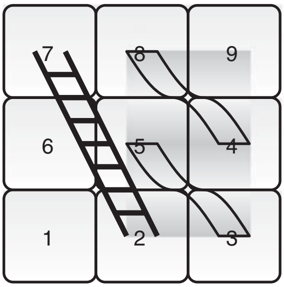

Figure 3.18

3.53 When an NFL football game ends in a tie, under *sudden-death* overtime the two teams play at most 15 extra minutes and the team that scores first wins the game. A Markov chain analysis of sudden-death is given in Jones (2004). Assuming two teams A and B are evenly matched, a four-state absorbing Markov chain is given with states PA: team A gains possession, PB: team B gains possession, A: A wins, and B: B wins. The transition matrix is

$$\boldsymbol{P} = \begin{array}{c} \\ PA \\ PB \\ A \\ B \end{array} \begin{array}{c} \begin{array}{cccc} PA & PB & A & B \end{array} \\ \begin{pmatrix} 0 & 1-p & p & 0 \\ 1-p & 0 & 0 & p \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array},$$

where p is the probability that a team scores when it has the ball. Which team first receives the ball in overtime is decided by a coin flip.

(a) If team A receives the ball in overtime, find the probability that A wins.

(b) An alternate overtime procedure is the *first-to-six rule*, where the first time to score six points in overtime wins the game. Consider two evenly matched teams. Let α be the probability that a team scores a touchdown (six points). Let β be the probability that a team scores a field goal (three points). Assume for simplicity that touchdowns and field goals are the only way points can be scored. Develop a 10-state Markov chain model for overtime play.

(c) For the 2002 regular NFL season, there were 6,049 possessions, 1,270 touchdowns, and 737 field goals. Using these data compare the probability that A wins the game for each of the two overtime procedures.

3.54 A mouse is placed in the maze in Figure 3.19 starting in box A. A piece of cheese is put in box I. From each room the mouse moves to an adjacent room through an open door, choosing from the available doors with equal probability.

(a) How many rooms, on average, will the mouse visit before it finds the cheese?

(b) How many times, on average, will the mouse visit room A before it finds the cheese?

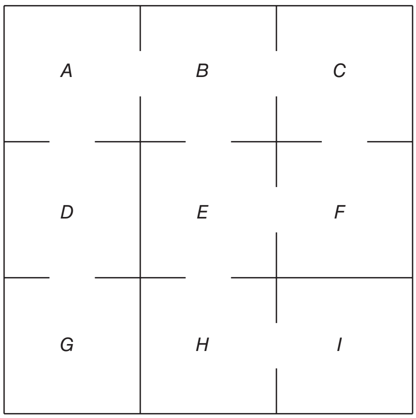

Figure 3.19 Mouse in a maze.

3.55 In a sequence of fair coin flips, how many flips, on average, are required to first see the pattern H-H-T-H?

3.56 A biased coin has heads probability 1/3 and tails probability 2/3. If the coin is tossed repeatedly, find the expected number of flips required until the pattern H-T-T-H-H appears.

3.57 In repeated coin flips, consider the set of all three-element patterns:

$$\{\text{HHH, HHT, HTH, HTT, THH, THT, TTH, TTT}\}.$$

Which patterns take the longest time, on average, to appear in repeated sampling? Which take the shortest?

3.58 A sequence of 0s and 1s is generated by a Markov chain with transition matrix

$$P = \begin{array}{c c} & \begin{array}{cc} 0 & 1 \end{array} \\ \begin{array}{c} 0 \\ 1 \end{array} & \begin{pmatrix} 1/4 & 3/4 \\ 3/4 & 1/4 \end{pmatrix} \end{array}.$$

The first element of the sequence is decided by a fair coin flip. On average, how many steps are required for the pattern 0-0-1-1 to first appear?

3.59 Consider random walk on the weighted graph in Figure 3.20.

(a) If the walk starts in a, find the expected number of steps to return to a.

(b) If the walk starts in a, find the expected number of steps to first hit b.

(c) If the walk starts in a, find the probability that the walk hits b before c.

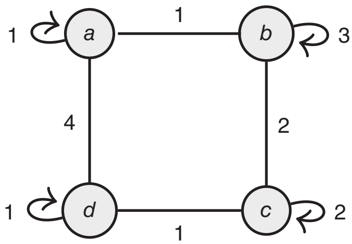

Figure 3.20

3.60 For a Markov chain started in state i, let T denote the *fifth time* the chain visits state i. Is T a stopping time? Explain.

3.61 Consider the weather Markov chain $X_0, X_1, \ldots$ of Example 2.3. Let T be the first time that it rains for 40 days in a row. Is $X_T, X_{T+1}, X_{T+2}, \ldots$ a Markov chain? Explain.

3.62 Let S be a random variable that is constant, with probability 1, where that constant is some positive integer. Show that S is a stopping time. Conclude that the Markov property follows from the strong Markov property.

3.63 `R` : Hourly wind speeds in a northwestern region of Turkey are modeled by a Markov chain in Sahin and Sen (2001). Seven wind speed levels are the states of the chain. The transition matrix is

$$P = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{array} \begin{array}{c} \begin{array}{ccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{array} \\ \begin{pmatrix} 0.756 & 0.113 & 0.129 & 0.002 & 0 & 0 & 0 \\ 0.174 & 0.821 & 0.004 & 0.001 & 0 & 0 & 0 \\ 0.141 & 0.001 & 0.776 & 0.082 & 0 & 0 & 0 \\ 0.003 & 0 & 0.192 & 0.753 & 0.052 & 0 & 0 \\ 0 & 0 & 0.002 & 0.227 & 0.735 & 0.036 & 0 \\ 0 & 0 & 0 & 0.007 & 0.367 & 0.604 & 0.022 \\ 0 & 0 & 0 & 0 & 0.053 & 0.158 & 0.789 \end{pmatrix} \end{array}.$$

(a) Find the limiting distribution by (i) taking high matrix powers, and (ii) using the `stationary` command in the **utilities.R** file. How often does the highest wind speed occur? How often does the lowest speed occur?

(b) Simulate the chain for 100,000 steps and estimate the proportion of times that the chain visits each state.

3.64 `R`: The evolution of forest ecosystems in the United States and Canada is studied in Strigul et al. (2012) using Markov chains. Five-year changes in the state of the forest soil are modeled with a 12-state Markov chain. The transition matrix can be found in the `R` script file **forest.R**. About how many years does it take for the ecosystem to move from state 1 to state 12?

3.65 `R`: Simulate the gambler's ruin problem for a gambler who starts with \$15 and quits when he reaches \$50 or goes bust. Use your code to simulate the probability of eventual ruin and compare to the exact probability.

3.66 `R`: Simulate the expected hitting time for the random walk on the hexagon in Exercise 3.19.

3.67 `R`: Simulate the dice game of Exercise 3.38. Verify numerically the theoretical expectation for the number of throws needed to get all sixes.

3.68 `R` : Write a function `reversal(mat)`, whose input is the transition matrix of an irreducible Markov chain and whose output is the transition matrix of the reversal chain.

3.69 `R` : Make up your own board game which can be modeled as a Markov chain. Ask interesting questions and answer them by simulation and/or an exact analysis.