Chapter 4
Markov Chains

4.1. Introduction

In this chapter, we consider a stochastic process $\{X_n, n = 0, 1, 2, \ldots\}$ that takes on a finite or countable number of possible values. Unless otherwise mentioned, this set of possible values of the process will be denoted by the set of nonnegative integers $\{0, 1, 2, \ldots\}$. If $X_n = i$, then the process is said to be in state i at time n. We suppose that whenever the process is in state i, there is a fixed probability P_{ij} that it will next be in state j. That is, we suppose that

$$P\{X_{n+1} = j \mid X_n = i, X_{n-1} = i_{n-1}, \ldots, X_1 = i_1, X_0 = i_0\} = P_{ij} \quad (4.1)$$

for all states $i_0, i_1, \ldots, i_{n-1}, i, j$ and all $n \geq 0$. Such a stochastic process is known as a ***Markov chain.*** Equation *(4.1)* may be interpreted as stating that, for a Markov chain, the conditional distribution of any future state X_{n+1} given the past states $X_0, X_1, \ldots, X_{n-1}$ and the present state X_n, is independent of the past states and depends only on the present state.

The value P_{ij} represents the probability that the process will, when in state i, next make a transition into state j. Since probabilities are nonnegative and since the process must make a transition into some state, we have that

$$P_{ij} \geq 0, \qquad i, j \geq 0; \qquad \sum_{j=0}^{\infty} P_{ij} = 1, \qquad i = 0, 1, \ldots$$

Let P denote the matrix of one-step transition probabilities P_{ij}, so that

$$\mathbf{P} = \begin{Vmatrix} P_{00} & P_{01} & P_{02} & \cdots \\ P_{10} & P_{11} & P_{12} & \cdots \\ \vdots & & & \\ P_{i0} & P_{i1} & P_{i2} & \cdots \\ \vdots & \vdots & \vdots & \end{Vmatrix}$$

Example 4.1 (Forecasting the Weather): Suppose that the chance of rain tomorrow depends on previous weather conditions only through whether or not it is raining today and not on past weather conditions. Suppose also that if it rains today, then it will rain tomorrow with probability α; and if it does not rain today, then it will rain tomorrow with probability β.

If we say that the process is in state 0 when it rains and state 1 when it does not rain, then the above is a two-state Markov chain whose transition probabilities are given by

$$\mathbf{P} = \begin{Vmatrix} \alpha & 1-\alpha \\ \beta & 1-\beta \end{Vmatrix} \quad \blacklozenge$$

Example 4.2 (A Communications System): Consider a communications system which transmits the digits 0 and 1. Each digit transmitted must pass through several stages, at each of which there is a probability p that the digit entered will be unchanged when it leaves. Letting X_n denote the digit entering the nth stage, then $\{X_n, n = 0, 1, \ldots\}$ is a two-state Markov chain having a transition probability matrix

$$\mathbf{P} = \begin{Vmatrix} p & 1-p \\ 1-p & p \end{Vmatrix} \quad \blacklozenge$$

Example 4.3 On any given day Gary is either cheerful (C), so-so (S), or glum (G). If he is cheerful today, then he will be C, S, or G tomorrow with respective probabilities 0.5, 0.4, 0.1. If he is feeling so-so today, then he will be C, S, or G tomorrow with probabilities 0.3, 0.4, 0.3. If he is glum today, then he will be C, S, or G tomorrow with probabilities 0.2, 0.3, 0.5.

Letting X_n denote Gary's mood on the nth day, then $\{X_n, n \geq 0\}$ is a three-state Markov chain (state 0 = C, state 1 = S, state 2 = G) with transition probability matrix

$$\mathbf{P} = \begin{Vmatrix} 0.5 & 0.4 & 0.1 \\ 0.3 & 0.4 & 0.3 \\ 0.2 & 0.3 & 0.5 \end{Vmatrix} \quad \blacklozenge$$

Example 4.4 (Transforming a Process into a Markov Chain): Suppose that whether or not it rains today depends on previous weather conditions through the last two days. Specifically, suppose that if it has rained for the past two days, then it will rain tomorrow with probability 0.7; if it rained today but not yesterday, then it will rain tomorrow with probability 0.5; if it rained yesterday but not today, then it will rain tomorrow with probability 0.4; if it has not rained in the past two days, then it will rain tomorrow with probability 0.2.

If we let the state at time n depend only on whether or not it is raining at time n, then the above model is not a Markov chain (why not?). However, we can transform the above model into a Markov chain by saying that the state at any time is determined by the weather conditions during both that day and the previous day. In other words, we can say that the process is in

state 0 if it rained both today and yesterday,
state 1 if it rained today but not yesterday,
state 2 if it rained yesterday but not today,
state 3 if it did not rain either yesterday or today.

The preceding would then represent a four-state Markov chain having a transition probability matrix

$$\mathbf{P} = \begin{Vmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{Vmatrix}$$

The reader should carefully check the matrix P, and make sure he or she understands how it was obtained. ◆

Example 4.5 (A Random Walk Model): A Markov chain whose state space is given by the integers $i = 0, \pm 1, \pm 2, \ldots$ is said to be a random walk if, for some number $0 < p < 1$,

$$p_{i,i+1} = p = 1 - P_{i,i-1}, \qquad i = 0, \pm 1, \ldots$$

The preceding Markov chain is called a random walk for we may think of it as being a model for an individual walking on a straight line who at each point of time either takes one step to the right with probability p or one step to the left with probability $1 - p$. ◆

Example 4.6 (A Gambling Model): Consider a gambler who, at each play of the game, either wins \$1 with probability p or loses \$1 with probability $1 - p$. If we suppose that our gambler quits playing either when he goes broke or he attains a fortune of \$N, then the gambler's fortune is a Markov chain having transition probabilities

$$P_{i,i+1} = p = 1 - P_{i,i-1}, \qquad i = 1, 2, \ldots, N-1$$
$$P_{00} = P_{NN} = 1$$

States 0 and N are called absorbing states since once entered they are never left. Note that the above is a finite state random walk with absorbing barriers (states 0 and N). ◆

4.2. Chapman-Kolmogorov Equations

We have already defined the one-step transition probabilities P_{ij}. We now define the n-step transition probabilities P_{ij}^n to be the probability that a process in state i will be in state j after n additional transitions. That is,

$$P_{ij}^n = P\{X_{n+m} = j \mid X_m = i\}, \qquad n \geq 0,\ i, j \geq 0$$

Of course $P_{ij}^1 = P_{ij}$. The Chapman-Kolmogorov equations provide a method for computing these n-step transition probabilities. These equations are

$$P_{ij}^{n+m} = \sum_{k=0}^{\infty} P_{ik}^n P_{kj}^m \qquad \text{for all } n, m \geq 0, \text{ all } i, j \tag{4.2}$$

and are most easily understood by noting that $P_{ik}^n P_{kj}^m$ represents the probability that starting in i the process will go to state j in $n + m$ transitions through a path which takes it into state k at the nth transition. Hence, summing over all intermediate states k yields the probability that the process will be in state j after $n + m$ transitions. Formally, we have

$$\begin{aligned}
P_{ij}^{n+m} &= P\{X_{n+m} = j \mid X_0 = i\} \\
&= \sum_{k=0}^{\infty} P\{X_{n+m} = j, X_n = k \mid X_0 = i\} \\
&= \sum_{k=0}^{\infty} P\{X_{n+m} = j \mid X_n = k, X_0 = i\} P\{X_n = k \mid X_0 = i\} \\
&= \sum_{k=0}^{\infty} P_{kj}^m P_{ik}^n
\end{aligned}$$

If we let $\mathbf{P}^{(n)}$ denote the matrix of n-step transition probabilities P_{ij}^n, then Equation (4.2) asserts that

$$\mathbf{P}^{(n+m)} = \mathbf{P}^{(n)} \cdot \mathbf{P}^{(m)}$$

where the dot represents matrix multiplication.* Hence, in particular,

$$\mathbf{P}^{(2)} = \mathbf{P}^{(1+1)} = \mathbf{P} \cdot \mathbf{P} = \mathbf{P}^2$$

and by induction

$$\mathbf{P}^{(n)} = \mathbf{P}^{(n-1+1)} = \mathbf{P}^{n-1} \cdot \mathbf{P} = \mathbf{P}^n$$

That is, the n-step transition matrix may be obtained by multiplying the matrix P by itself n times.

Example 4.7 Consider Example 4.1 in which the weather is considered as a two-state Markov chain. If $\alpha = 0.7$ and $\beta = 0.4$, then calculate the probability that it will rain four days from today given that it is raining today.

Solution: The one-step transition probability matrix is given by

$$\mathbf{P} = \begin{Vmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{Vmatrix}$$

Hence,

$$\mathbf{P}^{(2)} = \mathbf{P}^2 = \begin{Vmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{Vmatrix} \cdot \begin{Vmatrix} 0.7 & 0.3 \\ 0.4 & 0.6 \end{Vmatrix}$$

$$= \begin{Vmatrix} 0.61 & 0.39 \\ 0.52 & 0.48 \end{Vmatrix},$$

$$\mathbf{P}^{(4)} = (\mathbf{P}^2)^2 = \begin{Vmatrix} 0.61 & 0.39 \\ 0.52 & 0.48 \end{Vmatrix} \cdot \begin{Vmatrix} 0.61 & 0.39 \\ 0.52 & 0.48 \end{Vmatrix}$$

$$= \begin{Vmatrix} 0.5749 & 0.4251 \\ 0.5668 & 0.4332 \end{Vmatrix}$$

and the desired probability P_{00}^4 equals 0.5749. ◆

Example 4.8 Consider Example 4.4. Given that it rained on Monday and Tuesday, what is the probability that it will rain on Thursday?

* If A is an $N \times M$ matrix whose element in the ith row and jth column is a_{ij} and B is a $M \times K$ matrix whose element in the ith row and jth column is b_{ij}, then $A \cdot B$ is defined to be the $N \times K$ matrix whose element in the ith row and jth column is $\sum_{k=1}^{M} a_{ik} b_{kj}$.

Solution: The two-step transition matrix is given by

$$\mathbf{P}^{(2)} = \mathbf{P}^2 = \begin{Vmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{Vmatrix} \cdot \begin{Vmatrix} 0.7 & 0 & 0.3 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.4 & 0 & 0.6 \\ 0 & 0.2 & 0 & 0.8 \end{Vmatrix}$$

$$= \begin{Vmatrix} 0.49 & 0.12 & 0.21 & 0.18 \\ 0.35 & 0.20 & 0.15 & 0.30 \\ 0.20 & 0.12 & 0.20 & 0.48 \\ 0.10 & 0.16 & 0.10 & 0.64 \end{Vmatrix}$$

Since rain on Thursday is equivalent to the process being in either state 0 or state 1 on Thursday, the desired probability is given by $P_{00}^2 + P_{01}^2 = 0.49 + 0.12 = 0.61$. ◆

So far, all of the probabilities we have considered are conditional probabilities. For instance, P_{ij}^n is the probability that the state at time n is j *given* that the initial state at time 0 is i. If the unconditional distribution of the state at time n is desired, it is necessary to specify the probability distribution of the initial state. Let us denote this by

$$\alpha_i \equiv P\{X_0 = i\}, \qquad i \geq 0 \left(\sum_{i=0}^{\infty} \alpha_i = 1 \right)$$

All unconditional probabilities may be computed by conditioning on the initial state. That is,

$$P\{X_n = j\} = \sum_{i=0}^{\infty} P\{X_n = j \mid X_0 = i\} P\{X_0 = i\}$$

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

For instance, if $\alpha_0 = 0.4$, $\alpha_1 = 0.6$, in Example 4.7, then the (unconditional) probability that it will rain four days after we begin keeping weather records is

$$P\{X_4 = 0\} = 0.4P_{00}^4 + 0.6P_{10}^4$$

$$= (0.4)(0.5749) + (0.6)(0.5668)$$

$$= 0.5700$$

4.3. Classification of States

State j is said to be accessible from state i if $P_{ij}^n > 0$ for some $n \geq 0$. Note that this implies that state j is accessible from state i if and only if, starting in i, it is possible that the process will ever enter state j. This is true since if j is not accessible from i, then

$$\begin{aligned} P\{\text{ever enter } j \mid \text{start in } i\} &= P\left\{ \bigcup_{n=0}^{\infty} \{X_n = j\} \mid X_0 = i \right\} \\ &\leq \sum_{n=0}^{\infty} P\{X_n = j \mid X_0 = i\} \\ &= \sum_{n=0}^{\infty} P_{ij}^n \\ &= 0 \end{aligned}$$

Two states i and j that are accessible to each other are said to communicate, and we write $i \leftrightarrow j$.

Note that any state communicates with itself since, by definition,

$$P_{ii}^0 = P\{X_0 = i \mid X_0 = i\} = 1$$

The relation of communication satisfies the following three properties:

(i) State i communicates with state i, all $i \geq 0$.
(ii) If state i communicates with state j, then state j communicates with state i.
(iii) If state i communicates with state j, and state j communicates with state k, then state i communicates with state k.

Properties (i) and (ii) follow immediately from the definition of communication. To prove (iii) suppose that i communicates with j, and j communicates with k. Thus, there exists integers n and m such that $P_{ij}^n > 0$, $P_{jk}^m > 0$. Now by the Chapman–Kolmogorov equations, we have that

$$P_{ik}^{n+m} = \sum_{r=0}^{\infty} P_{ir}^n P_{rk}^m \geq P_{ij}^n P_{jk}^m > 0$$

Hence, state k is accessible from state i. Similarly, we can show that state i is accessible from state k. Hence, states i and k communicate.

Two states that communicate are said to be in the same class. It is an easy consequence of (i), (ii), and (iii) that any two classes of states are either identical or disjoint. In other words, the concept of communication divides the state space up into a number of separate classes. The Markov chain is said to be ***irreducible*** if there is only one class, that is, if all states communicate with each other.

Example 4.9 Consider the Markov chain consisting of the three states 0, 1, 2 and having transition probability matrix

$$\mathbf{P} = \begin{Vmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ 0 & \frac{1}{3} & \frac{2}{3} \end{Vmatrix}$$

It is easy to verify that this Markov chain is irreducible. For example, it is possible to go from state 0 to state 2 since

$$0 \rightarrow 1 \rightarrow 2$$

That is, one way of getting from state 0 to state 2 is to go from state 0 to state 1 (with probability $\frac{1}{2}$) and then go from state 1 to state 2 (with probability $\frac{1}{4}$). **4**

Example 4.10 Consider a Markov chain consisting of the four states 0, 1, 2, 3 and have a transition probability matrix

$$\mathbf{P} = \begin{Vmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

The classes of this Markov chain are (0, 1}, {2}, and (3). Note that while state 0 (or 1) is accessible from state 2, the reverse is not true. Since state 3 is an absorbing state, that is, $P_{33} = 1$, no other state is accessible from it. **4**

For any state i we let f_i denote the probability that, starting in state i, the process will ever reenter state i. State i is said to be ***recurrent*** if $f_i = 1$ and ***transient*** if $f_i < 1$.

Suppose that the process starts in state i and i is recurrent. Hence, with probability 1, the process will eventually reenter state i. However, by the definition of a Markov chain, it follows that the process will be starting over again when it reenters state i and, therefore, state i will eventually be visited again. Continual repetition of this argument leads to the conclusion that *if* ***state i is recurrent then, starting in state i, the process will reenter state i again and again and again—in fact, infinitely often.***

On the other hand, suppose that state i is transient. Hence, each time the process enters state i there will be a positive probability, namely, $1 - f_i$, that it will never again enter that state. Therefore, starting in state i, the probability that the process will be in state i for exactly n time periods equals $f_i^{n-1}(1 - f_i)$, $n \geq 1$. In other words, ***if state i is transient then, starting in state i, the number of time periods that the process will be in state i has a geometric distribution with finite mean*** $1/(1 - f_i)$.

From the preceding two paragraphs, it follows that ***state i is recurrent if and only if, starting in state i, the expected number of time periods that the process is in state i is infinite.*** But, letting

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

we have that $\sum_{n=0}^{\infty} I_n$ represents the number of periods that the process is in state i. Also,

$$\begin{aligned} E\left[\sum_{n=0}^{\infty} I_n \,\middle|\, X_0 = i\right] &= \sum_{n=0}^{\infty} E[I_n \mid X_0 = i] \\ &= \sum_{n=0}^{\infty} P\{X_n = i \mid X_0 = i\} \\ &= \sum_{n=0}^{\infty} P_{ii}^n \end{aligned}$$

We have thus proven the following.

Proposition 4.1 State i is

$$\text{recurrent if } \sum_{n=1}^{\infty} P_{ii}^n = \infty,$$

$$\textbf{transient if } \sum_{n=1}^{\infty} P_{ii}^n < \infty$$

The argument leading to the preceding proposition is doubly important because it also shows that a transient state will only be visited a finite number of times (hence the name transient). This leads to the conclusion that in a finite-state Markov chain not all states can be transient. To see this, suppose the states are $0, 1, \ldots, M$ and suppose that they are all transient. Then after a finite amount of time (say, after time T_0) state 0 will never be visited, and after a time (say, T_1) state 1 will never be visited, and after a time (say, T_2) state 2 will never be visited, etc. Thus, after a finite time $T = \max\{T_0, T_1, \ldots, T_M\}$ no states will be visited. But as the process must be in some state after time T we arrive at a contradiction, which shows that at least one of the states must be recurrent.

Another use of Proposition 4.1 is that it enables us to show that recurrence is a class property.

Corollary 4.2 If state i is recurrent, and state i communicates with state j, then state j is recurrent.

Proof To prove this we first note that, since state i communicates with state j, there exists integers k and m such that $P_{ij}^k > 0$, $P_{ji}^m > 0$. Now, for any integer n

$$P_{jj}^{m+n+k} \geq P_{ji}^m P_{ii}^n P_{ij}^k$$

This follows since the left side of the above is the probability of going from j to j in m + n + k steps, while the right side is the probability of going from j to j in m + n + k steps via a path that goes from j to i in m steps, then from i to i in an additional n steps, then from i to j in an additional k steps.

From the preceding we obtain, by summing over n, that

$$\sum_{n=1}^{\infty} P_{jj}^{m+n+k} \geq P_{ji}^m P_{ij}^k \sum_{n=1}^{\infty} P_{ii}^n = \infty$$

since $P_{ji}^m P_{ij}^k > 0$, and $\sum_{n=1}^{\infty} P_{ii}^n$ is infinite since state i is recurrent. Thus, by Proposition 4.1 it follows that state j is also recurrent. ◆

Remarks (i) Corollary 4.2 also implies that transience is a class property. For if state i is transient and communicates with state j, then state j must also be transient. For if j were recurrent then, by Corollary 4.2, i would also be recurrent and hence could not be transient.

(ii) Corollary 4.2 along with our previous result that not all states in a finite Markov chain can be transient leads to the conclusion that all states of a finite irreducible Markov chain are recurrent.

Example 4.11 Let the Markov chain consisting of the states 0, 1, 2, 3 have the transition probability matrix

$$\mathbf{P} = \begin{Vmatrix} 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{Vmatrix}$$

Determine which states are transient and which are recurrent.

Solution: It is a simple matter to check that all states communicate and hence, since this is a finite chain, all states must be recurrent. ◆

Example 4.12 Consider the Markov chain having states 0, 1, 2, 3, 4 and

$$\mathbf{P} = \begin{Vmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{4} & 0 & 0 & \frac{1}{2} \end{Vmatrix}$$

Determine the recurrent state.

Solution: This chain consists of the three classes {0, 1}, {2, 3}, and (4). The first two classes are recurrent and the third transient. ◆

Example 4.13 (A Random Walk): Consider a Markov chain whose state space consists of the integers i = 0, ±1, ±2, ..., and have transition probabilities given by

$$P_{i,i+1} = p = 1 - P_{i,i-1}, \qquad i = 0, \pm 1, \pm 2, \ldots$$

where $0 < p < 1$. In other words, on each transition the process either moves one step to the right (with probability p) or one step to the left (with probability $1 - p$). One colorful interpretation of this process is that it represents the wanderings of a drunken man as he walks along a straight line. Another is that it represents the winnings of a gambler who on each play of the game either wins or loses one dollar.

Since all states clearly communicate, it follows from Corollary 4.2 that they are either all transient or all recurrent. So let us consider state 0 and attempt to determine if $\sum_{n=1}^{\infty} P_{00}^{n}$ is finite or infinite.

Since it is impossible to be even (using the gambling model interpretation) after an odd number of plays we must, of course, have that

$$P_{00}^{2n-1} = 0, \qquad n = 1, 2, \ldots$$

On the other hand, we would be even after 2n trials if and only if we won n of these and lost n of these. Because each play of the game results in a win with probability p and a loss with probability $1 - p$, the desired probability is thus the binomial probability

$$P_{00}^{2n} = \binom{2n}{n} p^n (1-p)^n = \frac{(2n)!}{n!n!}(p(1-p))^n, \qquad n = 1, 2, 3, \ldots$$

By using an approximation, due to Stirling, which asserts that

$$n! \sim n^{n+1/2} e^{-n} \sqrt{2\pi}, \tag{4.3}$$

where we say that $a_n \sim b_n$ when $\lim_{n\to\infty} a_n/b_n = 1$, we obtain

$$P_{00}^{2n} \sim \frac{(4p(1-p))^n}{\sqrt{\pi n}}$$

Now it is easy to verify that if $a_n \sim b_n$, then $\sum_n a_n < \infty$ if and only if $\sum_n b_n < \infty$. Hence, $\sum_{n=1}^{\infty} P_{00}^n$ will converge if and only if

$$\sum_{n=1}^{\infty} \frac{(4p(1-p))^n}{\sqrt{\pi n}}$$

does. However, $4p(1-p) \le 1$ with equality holding if and only if $p = \frac{1}{2}$. Hence, $\sum_{n=1}^{\infty} P_{00}^n = \infty$ if and only if $p = \frac{1}{2}$. Thus, the chain is recurrent when $p = \frac{1}{2}$ and transient if $p \neq \frac{1}{2}$.

When $p = \frac{1}{2}$, the above process is called a symmetric random walk. We could also look at symmetric random walks in more than one dimension. For instance, in the two-dimensional symmetric random walk the process would, at each transition, either take one step to the left, right, up, or down, each having probability $\frac{1}{4}$. That is, the state is the pair of integers (i, j) and the transition probabilities are given by

$$P_{(i,j),(i+1,j)} = P_{(i,j),(i-1,j)} = P_{(i,j),(i,j+1)} = P_{(i,j),(i,j-1)} = \tfrac{1}{4}$$

By using the same method as in the one-dimensional case, we now show that this Markov chain is also recurrent.

Since the preceding chain is irreducible, it follows that all states will be recurrent if state $0 = (0, 0)$ is recurrent. So consider P_{00}^{2n}. Now after $2n$ steps, the chain will be back in its original location if for some i, $0 \le i \le n$, the $2n$ steps consist of i steps to the left, i to the right, $n - i$ up, and $n - i$ down. Since each step will be either of these four types with probability $\frac{1}{4}$, it follows that the desired probability is a multinomial probability. That is,

$$\begin{aligned} P_{00}^{2n} &= \sum_{i=0}^{n} \frac{(2n)!}{i!\,i!\,(n-i)!\,(n-i)!} \left(\frac{1}{4}\right)^{2n} \\ &= \sum_{i=0}^{n} \frac{(2n)!}{n!\,n!} \frac{n!}{(n-i)!\,i!} \frac{n!}{(n-i)!\,i!} \left(\frac{1}{4}\right)^{2n} \\ &= \left(\frac{1}{4}\right)^{2n} \binom{2n}{n} \sum_{i=0}^{n} \binom{n}{i}\binom{n}{n-i} \\ &= \left(\frac{1}{4}\right)^{2n} \binom{2n}{n}\binom{2n}{n} \end{aligned} \tag{4.4}$$

where the last equality uses the combinatorial identity

$$\binom{2n}{n} = \sum_{i=0}^{n} \binom{n}{i}\binom{n}{n-i}$$

which follows upon noting that both sides represent the number of subgroups of size n one can select from a set of n white and n black objects. Now,

$$\begin{aligned}\binom{2n}{n} &= \frac{(2n)!}{n!n!}\\ &\sim \frac{(2n)^{2n+1/2}e^{-2n}\sqrt{2\pi}}{n^{2n+1}e^{-2n}(2\pi)} \qquad \text{by Stirling's approximation}\\ &= \frac{4^n}{\sqrt{\pi n}}\end{aligned}$$

Hence, from Equation (4.4) we see that

$$P_{00}^{2n} \sim \frac{1}{\pi n}$$

which shows that $\Sigma_n P_{00}^{2n} = \infty$, and thus all states are recurrent.

Interestingly enough, whereas the symmetric random walks in one and two dimensions are both recurrent, all high-dimensional symmetric random walks turn out to be transient. (For instance, the three-dimensional symmetric random walk is at each transition equally likely to move in any of six ways—either to the left, right, up, down, in, or out.) ◆

Remark We can compute the probability of whether the one-dimensional random walk of Example 4.13 ever returns to state 0 when $p \neq 1/2$ by conditioning on the initial transition:

$$\begin{aligned}P\{\text{ever return}\} = P\{&\text{ever return} \mid X_1 = 1\}p\\ &+ P\{\text{ever return} \mid X_1 = -1\}(1 - p)\end{aligned}$$

Suppose that $p > 1/2$. Then it can be shown (see Exercise 11 at the end of this chapter) that $P\{\text{ever return} \mid X_1 = -1\} = 1$, and thus

$$P\{\text{ever return}\} = P\{\text{ever return} \mid X_1 = 1\}p + 1 - p \tag{4.5}$$

Let $\alpha = P\{\text{ever return} \mid X_1 = 1\}$. Conditioning on the next transition gives

$$\begin{aligned}a &= P\{\text{ever return} \mid X_1 = 1, X_2 = 0\}(1 - p)\\ &\quad + P\{\text{ever return} \mid X_1 = 1, X_2 = 2\}p\\ &= 1 - p + P\{\text{ever enter } 0 \mid X_0 = 2\}p\end{aligned}$$

Now, if the chain is at state 2 then in order for it to enter state 0 it must first enter state 1 and the probability that this ever occurs is α (why is that?). Also, if it does enter state 1 then the probability that it ever enters state 0 is also a. Thus, we see that the probability of ever entering state 0 starting at state 2 is α^2. Therefore, we have that

$$\alpha = 1 - p + p\alpha^2$$

The two roots of this equation are $\alpha = 1$ and $a = (1 - p)/p$. The first is impossible since we know by transience that $a < 1$. Hence, $a = (1 - p)/p$, and we obtain from Equation (4.5) that

$$P\{\text{ever return}) = 1 - p + 1 - p = 2(1 - p)$$

Similarly, when $p < 1/2$ we can show that $P\{\text{ever return}) = 2p$. Thus, in general we have that

$$P\{\text{ever return}) = 2\min(p, 1 - p)$$

Example 4.14 (On the Ultimate Instability of the Aloha Protocol): Consider a communications facility in which the numbers of messages arriving during each of the time periods $n = 1, 2, \ldots$ are independent and identically distributed random variables. Let $a_i = P(i \text{ arrivals})$, and suppose that $a_0 + a, < 1$. Each arriving message will transmit at the end of the period in which it arrives. If exactly one message is transmitted, then the transmission is successful and the message leaves the system. However, if at any time two or more messages simultaneously transmit, then a collision is deemed to occur and these messages remain in the system. Once a message is involved in a collision it will, independently of all else, transmit at the end of each additional period with probability p—the so-called Aloha protocol (because it was first instituted at the University of Hawaii). We will show that such a system is asymptotically unstable in the sense that the number of successful transmissions will, with probability 1, be finite.

To begin let X_n denote the number of messages in the facility at the beginning of the nth period, and note that $\{X_n, n \geq 0\}$ is a Markov chain. Now for $k \geq 0$ define the indicator variables I_k by

$$I_k = \begin{cases} 1, & \text{if the first time that the chain departs state k it} \\ & \text{directly goes to state } k - 1 \\ 0, & \text{otherwise} \end{cases}$$

and let it be 0 if the system is never in state k, $k \geq 0$. (For instance, if the successive states are $0, 1, 3, 3, 4, \ldots$, then $I_3 = 0$ since when the chain first departs state 3 it goes to state 4; whereas, if they are $0, 3, 3, 2, \ldots$, then $I_3 = 1$ since this time it goes to state 2.) Now,

$$\begin{aligned} E\left[\sum_{k=0}^{\infty} I_k\right] &= \sum_{k=0}^{\infty} E[I_k] \\ &= \sum_{k=0}^{\infty} P\{I_k = 1\} \\ &\leq \sum_{k=0}^{w} P\{I_k = 1 \mid \text{k is ever visited}) \end{aligned} \tag{4.6}$$

Now, $P\{I_k = 1 \mid$ k is ever visited) is the probability that when state k is departed the next state is k $-$ 1. That is, it is the conditional probability that a transition from k is to k $-$ 1 given that it is not back into k, and so

$$P\{I_k = 1 \mid \text{k is ever visited}) = \frac{P_{k,k-1}}{1 - P_{kk}}.$$

As

$$P_{k,k-1} = a_0 kp(1 - p)^{k-1}$$
$$P_{k,k} = a_0[1 - kp(1 - p)^{k-1}] + a_1(1 - p)^k$$

which is seen by noting that if there are k messages present on the beginning of a day, then (a) there will be k $-$ 1 at the beginning of the next day if there are no new messages that day and exactly one of the k messages transmits; and (b) there will be k at the beginning of the next day if either

(i) there are no new messages and it is not the case that exactly one of the existing k messages transmits, or
(ii) there is exactly one new message (which automatically transmits) and none of the other k messages transmits.

Substitution of the preceding into Equation (4.6) yields

$$E\left[\sum_{k=0}^{\infty} I_k\right] \leq \sum_{k=0}^{\infty} \frac{a_0 kp(1 - p)^{k-1}}{1 - a_0[1 - kp(1 - p)^{k-1}] - a_1(1 - p)^k}$$
$$< \infty$$

where the convergence follows by noting that when k is large the denominator of the expression in the preceding sum converges to $1 - a_0$ and so the convergence or divergence of the sum is determined by whether or not the sum of the terms in the numerator converge and $\sum_{k=,}^{\infty} \mathrm{k}(1 - p)^{k-1} < \infty$.

Hence, $\mathrm{E}[\sum_{k=0}^{\infty} I_k] < \infty$, which implies that $\sum_{k=0}^{\infty} I_k < \infty$ with probability 1 (for if there was a positive probability that $\sum_{k=0}^{\infty} I_k$ could be ∞, then its mean would be m). Hence, with probability 1, there will be only a finite number of states that are initially departed via a successful transmission; or equivalently, there will be some finite integer N such that whenever there are N or more messages in the system, there will never again be a successful transmission. From this (and the fact that such higher states will eventually be reached—why?) it follows that, with probability 1, there will only be a finite number of successful transmissions. ◆

Remark For a (slightly less than rigorous) probabilistic proof of Stirling's approximation, let $X_1, X_2, \ldots$ be independent Poisson random variables each having mean 1. Let $S_n = \sum_{i=1}^{n} X_i$, and note that both the mean and variance of S_n are equal to n. Now,

$$\begin{aligned} P\{S_n = n\} &= P\{n - 1 < S_n \le n\} \\ &= P\{-1/\sqrt{n} < (S_n - n)/\sqrt{n} \le 0\} \\ &\approx \int_{-1/\sqrt{n}}^{0} (2\pi)^{-1/2} e^{-x^2/2}\, dx \quad \text{when n is large, by the central limit theorem} \\ &\approx (2\pi)^{-1/2}(1/\sqrt{n}) \\ &= (2\pi n)^{-1/2} \end{aligned}$$

But S_n is Poisson with mean n, and so

$$P\{S_n = n\} = \frac{e^{-n} n^n}{n!}$$

Hence, for n large

$$\frac{e^{-n} n^n}{n!} \approx (2\pi n)^{-1/2}$$

or, equivalently

$$n! \approx n^{n+1/2} e^{-n} \sqrt{2\pi}$$

which is **Stirling's** approximation.

4.4. Limiting Probabilities

In Example 4.7, we calculated $\mathbf{P}^{(4)}$ for a two-state Markov chain; it turned out to be

$$\mathbf{P}^{(4)} = \begin{Vmatrix} 0.5749 & 0.4251 \\ 0.5668 & 0.4332 \end{Vmatrix}$$

From this it follows that $\mathbf{P}^{(8)} = \mathbf{P}^{(4)} \cdot \mathbf{P}^{(4)}$ is given (to three significant places) by

$$\mathbf{P}^{(8)} = \begin{Vmatrix} 0.572 & 0.428 \\ 0.570 & 0.430 \end{Vmatrix}$$

Note that the matrix $\mathbf{P}^{(8)}$ is almost identical to the matrix $\mathbf{P}^{(4)}$, and secondly, that each of the rows of $\mathbf{P}^{(8)}$ has almost identical entries. In fact it seems that P_{ij}^n is converging to some value (as $n \to \infty$) which is the same for all i. In other words, there seems to exist a limiting probability that the process will be in state j after a large number of transitions, and this value is independent of the initial state.

To make the above heuristics more precise there are two additional properties of the states of a Markov chain that we need consider. State i is said to have period d if $P_{ii}^n = 0$ whenever n is not divisible by d, and d is the largest integer with this property. For instance, starting in i, it may be possible for the process to enter state i only at the times 2, 4, 6, 8, ..., in which case state i has period 2. A state with period 1 is said to be aperiodic. It can be shown that periodicity is a class property. That is, if state i has period d, and states i and j communicate, then state j also has period d.

If state i is recurrent, then it is said to be *positive recurrent* if, starting in i, the expected time until the process returns to state i is finite. It can be shown that positive recurrence is a class property. While there exist recurrent states that are not positive recurrent,* it can be shown that in *a finite-state* Markov chain all recurrent states are positive recurrent. Positive recurrent, aperiodic states are called ergodic.

We are now ready for the following important theorem which we state without proof.

Theorem 4.1 For an irreducible ergodic Markov chain $\lim_{n\to\infty} P_{ij}^n$ exists and is independent of i. Furthermore, letting

$$\pi_j = \lim_{n\to\infty} P_{ij}^n, \qquad j \geq 0$$

then π_j is the unique nonnegative solution of

$$\begin{aligned} \pi_j &= \sum_{i=0}^{\infty} \pi_i P_{ij}, \qquad j \geq 0 \\ \sum_{j=0}^{\infty} \pi_j &= 1 \end{aligned} \tag{4.7}$$

Remarks (i) Given that $\pi_j = \lim_{n\to\infty} P_{ij}^n$ exists and is independent of the initial state i, it is not difficult to (heuristically) see that the π's must satisfy Equation (4.7). For let us derive an expression for $P\{X_{n+1} = j\}$ by conditioning on the state at time n. That is,

$$\begin{aligned} P\{X_{n+1} = j\} &= \sum_{i=0}^{\infty} P\{X_{n+1} = j \mid X_n = i\} P\{X_n = i\} \\ &= \sum_{i=0}^{\infty} P_{ij} P\{X_n = i\} \end{aligned}$$

* Such states are called *null recurrent.*

Letting $n \to \infty$, and assuming that we can bring the limit inside the summation, leads to

$$\pi_j = \sum_{i=0}^{\infty} P_{ij}\pi_i$$

(ii) It can be shown that π_j, the limiting probability that the process will be in state j at time n, also equals the long-run proportion of time that the process will be in state j.

(iii) In the irreducible, positive recurrent, *periodic* case we still have that the π_j, $j \geq 0$, are the unique nonnegative solution of

$$\pi_j = \sum_i \pi_i P_{ij},$$
$$\sum_j \pi_j = 1$$

But now π_j must be interpreted as the long-run proportion of time that the Markov chain is in state j.

Example 4.15 Consider Example 4.1, in which we assume that if it rains today, then it will rain tomorrow with probability α; and if it does not rain today, then it will rain tomorrow with probability β. If we say that the state is 0 when it rains and 1 when it does not rain, then by Equation (4.7) the limiting probabilities π_0 and π_1 are given by

$$\pi_0 = \alpha\pi_0 + \beta\pi_1,$$
$$\pi_1 = (1 - \alpha)\pi_0 + (1 - \beta)\pi_1,$$
$$\pi_0 + \pi_1 = 1$$

which yields that

$$\pi_0 = \frac{\beta}{1 + \beta - \alpha}, \qquad \pi_1 = \frac{1 - \alpha}{1 + \beta - \alpha}$$

For example if $\alpha = 0.7$ and $\beta = 0.4$, then the limiting probability of rain is $\pi_0 = \frac{4}{7} = 0.571$. ◆

Example 4.16 Consider Example 4.3 in which the mood of an individual is considered as a three-state Markov chain having a transition probability matrix

$$\mathbf{P} = \begin{Vmatrix} 0.5 & 0.4 & 0.1 \\ 0.3 & 0.4 & 0.3 \\ 0.2 & 0.3 & 0.5 \end{Vmatrix}$$

In the long run, what proportion of time is the process in each of the three states?

Solution: The limiting probabilities π_i, i = 0, 1, 2, are obtained by solving the set of equations in Equation (4.1). In this case these equations are

$$\pi_0 = 0.5\pi_0 + 0.3\pi_1 + 0.2\pi_2,$$
$$\pi_1 = 0.4\pi_0 + 0.4\pi_1 + 0.3\pi_2,$$
$$\pi_2 = 0.1\pi_0 + 0.3\pi_1 + 0.5\pi_2,$$
$$\pi_0 + \pi_1 + \pi_2 = 1$$

Solving yields

$$\pi_0 = \tfrac{21}{62}, \qquad \pi_1 = \tfrac{23}{62}, \qquad \pi_2 = \tfrac{18}{62} \quad \blacklozenge$$

Example 4.17 (A Model of Class Mobility): A problem of interest to sociologists is to determine the proportion of society that has an upper- or lower-class occupation. One possible mathematical model would be to assume that transitions between social classes of the successive generations in a family can be regarded as transitions of a Markov chain. That is, we assume that the occupation of a child depends only on his or her parent's occupation. Let us suppose that such a model is appropriate and that the transition probability matrix is given by

$$\mathbf{P} = \begin{Vmatrix} 0.45 & 0.48 & 0.07 \\ 0.05 & 0.70 & 0.25 \\ 0.01 & 0.50 & 0.49 \end{Vmatrix} \tag{4.8}$$

That is, for instance, we suppose that the child of a middle-class worker will attain an upper-, middle-, or lower-class occupation with respective probabilities 0.05, 0.70, 0.25.

The limiting probabilities π_i, thus satisfy

$$\pi_0 = 0.45\pi_0 + 0.05\pi_1 + 0.01\pi_2,$$
$$\pi_1 = 0.48\pi_0 + 0.70\pi_1 + 0.50\pi_2,$$
$$\pi_2 = 0.07\pi_0 + 0.25\pi_1 + 0.49\pi_2,$$
$$\pi_0 + \pi_1 + \pi_2 = 1$$

Hence,

$$\pi_0 = 0.07, \qquad \pi_1 = 0.62, \qquad \pi_2 = 0.31$$

In other words, a society in which social mobility between classes can be described by a Markov chain with transition probability matrix given by Equation (4.8) has, in the long run, 7 percent of its people in upper-class jobs, 62 percent of its people in middle-class jobs, and 31 percent in lower-class jobs. +

Example 4.18 (The Hardy–Weinberg Law and a Markov Chain in Genetics): Consider a large population of individuals each of whom possesses a particular pair of genes, of which each individual gene is classified as being of type A or type a. Assume that the proportions of individuals whose gene pairs are AA, aa, or Aa are respectively p_0, q_0, and r_0 ($p_0 + q_0 + r_0 = 1$). When two individuals mate, each contributes one of his or her genes, chosen at random, to the resultant offspring. Assuming that the mating occurs at random, in that each individual is equally likely to mate with any other individual, we are interested in determining the proportions of individuals in the next generation whose genes are AA, aa, or Aa. Calling these proportions p, q, and r, they are easily obtained by focusing attention on an individual of the next generation and then determining the probabilities for the gene pair of that individual.

To begin, note that randomly choosing a parent and then randomly choosing one of its genes is equivalent to just randomly choosing a gene from the total gene population. By conditioning on the gene pair of the parent, we see that a randomly chosen gene will be type A with probability

$$\begin{aligned} P\{A\} &= P\{A \mid AA\}p_0 + P\{A \mid aa\}q_0 + P\{A \mid Aa\}r_0 \\ &= p_0 + r_0/2 \end{aligned}$$

Similarly, it will be type a with probability

$$P\{a\} = q_0 + r_0/2$$

Thus, under random mating a randomly chosen member of the next generation will be type AA with probability p, where

$$p = P\{A\}P\{A\} = (p_0 + r_0/2)^2$$

Similarly, the randomly chosen member will be type aa with probability

$$q = P\{a\}P\{a\} = (q_0 + r_0/2)^2$$

and will be type Aa with probability

$$r = 2P\{A\}P\{a\} = 2(p_0 + r_0/2)(q_0 + r_0/2)$$

Since each member of the next generation will independently be of each of the three gene types with probabilities p, q, r, it follows that the percentages of the members of the next generation that are of type AA, aa, or Aa are respectively p, q, and r.

If we now consider the total gene pool of this next generation, then $p + r/2$, the fraction of its genes that are A, will be unchanged from the previous generation. This follows either by arguing that the total gene pool has not changed from generation to generation or by the following simple algebra:

$$\begin{aligned} p + r/2 &= (p_0 + r_0/2)^2 + (p_0 + r_0/2)(q_0 + r_0/2) \\ &= (p_0 + r_0/2)[p_0 + r_0/2 + q_0 + r_0/2] \\ &= p_0 + r_0/2 \qquad \text{since } p_0 + r_0 + q_0 = 1 \\ &= P\{A\} \end{aligned} \tag{4.9}$$

Thus, the fractions of the gene pool that are A and a are the same as in the initial generation. From this it follows that, under random mating, in all successive generations after the initial one the percentages of the population having gene pairs AA, aa, and Aa will remain fixed at the values p, q, and r. This is known as the Hardy-*Weinberg* law. ◆

Suppose now that the gene pair population has stabilized in the percentages p, q, r, and let us follow the genetic history of a single individual and her descendants. (For simplicity, assume that each individual has exactly one offspring.) So, for a given individual, let X_n denote the genetic state of her descendant in the nth generation. The transition probability matrix of this Markov chain, namely,

$$\begin{array}{c} \\ AA \\ \\ aa \\ \\ Aa \end{array} \begin{array}{c} \begin{array}{ccc} AA & aa & Aa \end{array} \\ \left\| \begin{array}{ccc} p + \dfrac{r}{2} & 0 & q + \dfrac{r}{2} \\ 0 & q + \dfrac{r}{2} & p + \dfrac{r}{2} \\ \dfrac{p}{2} + \dfrac{r}{4} & \dfrac{q}{2} + \dfrac{r}{4} & \dfrac{p}{2} + \dfrac{q}{2} + \dfrac{r}{2} \end{array} \right\| \end{array}$$

is easily verified by conditioning on the state of the randomly chosen mate. It is quite intuitive (why?) that the limiting probabilities for this Markov chain (which also equal the fractions of the individual's descendants that are in each of the three genetic states) should just be p, q, and r. To verify this we must show that they satisfy Equation (4.7). As one of the equations in Equation (4.7) is redundant, it suffices to show that

$$p = p\left(p + \frac{r}{2}\right) + r\left(\frac{p}{2} + \frac{r}{4}\right) = \left(p + \frac{r}{2}\right)^2,$$

$$q = q\left(q + \frac{r}{2}\right) + r\left(\frac{q}{2} + \frac{r}{4}\right) = \left(q + \frac{r}{2}\right)^2,$$

$$p + q + r = 1$$

But this follows from Equation **(4.9),** and thus the result is established.

Example 4.19 Suppose that a production process changes states in accordance with a Markov chain having transition probabilities P_{ij}, $i, j = 1, \ldots, n$, and suppose that certain of the states are considered acceptable and the remaining unacceptable. Let A denote the acceptable states and A^c the unacceptable ones. If the production process is said to be "up" when in an acceptable state and "down" when in an unacceptable state, determine

1. the rate at which the production process goes from up to down (that is, the rate of breakdowns);
2. the average length of time the process remains down when it goes down; and
3. the average length of time the process remains up when it goes up.

Solution: Let π_k, $k = 1, \ldots, n$, denote the limiting probabilities. Now for $i \in A$ and $j \in A^c$ the rate at which the process enters state j from state i is

$$\text{rate enter } j \text{ from } i = \pi_i P_{ij}$$

and so the rate at which the production process enters state j from an acceptable state is

$$\text{rate enter } j \text{ from } A = \sum_{i \in A} \pi_i P_{ij}$$

Hence, the rate at which it enters an unacceptable state from an acceptable one (which is the rate at which breakdowns occur) is

$$\text{rate breakdowns occur} = \sum_{j \in A^c} \sum_{i \in A} \pi_i P_{ij} \tag{4.10}$$

Now let $\bar{U}$ and $\bar{D}$ denote the average time the process remains up when it goes up and down when it goes down. Because there is a single breakdown every $\bar{U} + \bar{D}$ time units on the average, if follows heuristically that

$$\text{rate at which breakdowns occur} = \frac{1}{\bar{U} + \bar{D}}$$

and, so from Equation (4.10),

$$\frac{1}{\bar{U} + \bar{D}} = \sum_{j \in A^c} \sum_{i \in A} \pi_i P_{ij} \tag{4.11}$$

To obtain a second equation relating $\bar{U}$ and D, consider the percentage of time the process is up, which, of course, is equal to $\sum_{i \in A} \pi_i$. However, since the process is up on the average $\bar{U}$ out of every $\bar{U}$ + D time units, it follows (again somewhat heuristically) that the

$$\text{proportion of up time} = \frac{\bar{U}}{O+d}$$

and so

$$\frac{\bar{U}}{\bar{U} + \bar{D}} = \sum_{i \in A} \pi_i \tag{4.12}$$

Hence, from Equations (4.11) and (4.12) we obtain

$$\bar{U} = \frac{\sum_{i \in A} \pi_i}{\sum_{j \in A^c} \sum_{i \in A} \pi_i P_{ij}},$$

$$\bar{D} = \frac{1 - \sum_{i \in A} \pi_i}{\sum_{j \in A^c} \sum_{i \in A} \pi_i P_{ij}}$$

$$= \frac{\sum_{i \in A^c} \pi_i}{\sum_{j \in A^c} \sum_{i \in A} \pi_i P_{ij}}$$

For example, suppose the transition probability matrix is

$$\mathbf{P} = \begin{Vmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & 0 & \frac{1}{2} \end{Vmatrix}$$

where the acceptable (up) states are 1, 2 and the unacceptable (down) ones are 3, 4. The limiting probabilities satisfy

$$\pi_1 = \pi_1 \tfrac{1}{4} + \pi_3 \tfrac{1}{4} + \pi_4 \tfrac{1}{4},$$

$$\pi_2 = \pi_1 \tfrac{1}{4} + \pi_2 \tfrac{1}{4} + \pi_3 \tfrac{1}{4} + \pi_4 \tfrac{1}{4},$$

$$\pi_3 = \pi_1 \tfrac{1}{2} + \pi_2 \tfrac{1}{2} + \pi_3 \tfrac{1}{4},$$

$$\pi_1 + \pi_2 + \pi_3 + \pi_4 = 1$$

These solve to yield

$$\pi_1 = \tfrac{3}{16}, \qquad \pi_2 = \tfrac{1}{4}, \qquad \pi_3 = \tfrac{14}{48}, \qquad \pi_4 = \tfrac{13}{48}$$

and thus

$$\begin{aligned} \text{Rate of breakdowns} &= \pi_1(P_{13} + P_{14}) + \pi_2(P_{23} + P_{24}) \\ &= \tfrac{9}{32}, \\ \bar{U} = \tfrac{14}{9} \quad &\text{and} \quad \bar{D} = 2 \end{aligned}$$

Hence, on the average, breakdowns occur about $\frac{9}{32}$ (or 28 percent) of the time. They last, on the average, 2 time units, and then there follows a stretch of (on the average) $\frac{14}{9}$ time units when the system is up. ◆

Remarks (i) The long run proportions π_j, $j \geq 0$, are often called stationary probabilities. The reason being that if the initial state is chosen according to the probabilities π_j, $j \geq 0$, then the probability of being in state j at any time n is also equal to π_j. That is, if

$$P\{X_0 = j\} = \pi_j, \qquad j \geq 0$$

then

$$P\{X_n = j\} = \pi_j \qquad \text{for all } n, j \geq 0$$

The preceding is easily proven by induction, for if we suppose it true for $n - 1$, then writing

$$\begin{aligned} P\{X_n = j\} &= \sum_i P\{X_n = j \mid X_{n-1} = i\}P\{X_{n-1} = i\} \\ &= \sum_i P_{ij}\pi_i \qquad \text{by the induction hypothesis} \\ &= \pi_j \qquad \text{by Equation (4.7)} \end{aligned}$$

(ii) For state j, define m_{jj} to be the expected number of transitions until a Markov chain, starting in state j, returns to that state. Since, on the average, the chain will spend 1 unit of time in state j for every m_{jj} units of time, it follows that

$$\pi_j = \frac{1}{m_{jj}}$$

In words, the proportion of time in state j equals the inverse of the mean time between visits to j. (The above is a special case of a general result, sometimes called the strong law for renewal processes, which will be presented in Chapter 7.)

Example 4.20 Consider independent tosses of a coin that, on each toss, lands on heads (H) with probability p and on tails (T) with probability $q = 1 - p$. What is the expected number of tosses needed for the pattern HTHT to appear?

Solution: To answer the question, let us imagine that the coin tossing does not stop when the pattern appears, but rather it goes on indefinitely. If we define the state at time n to be the most recent 4 outcomes when $n \geq 4$, and the most recent n outcomes when $n < 4$, then it is easy to see that the successive states constitute a Markov chain. For instance, if the first 5 outcomes are TTTHH, then the successive states of the Markov chain are $X_1 = \text{T}$, $X_2 = \text{TT}$, $X_3 = \text{TTT}$, $X_4 = \text{TTTH}$, and $X_5 = \text{TTHH}$. It therefore follows from remark (ii) that π_{HTHT}, the limiting probability of state HTHT, is equal to the inverse of the mean time to go from state HTHT to HTHT. However, for any $n \geq 4$, the probability that the state at time n is HTHT is just the probability that the toss at n is T, the one at $n - 1$ is H, the one at $n - 2$ is T, and the one at $n - 3$ is H. Since the successive tosses are independent, it follows that

$$P\{X_n = \text{HTHT}) = p^2q^2, \qquad n \geq 4$$

and so

$$\pi_{\text{HTHT}} = \lim_{n\to\infty} P\{X_n = \text{HTHT}\} = p^2q^2$$

Hence, $1/(p^2q^2)$ is the mean time to go from HTHT to HTHT. But this means that starting with HT the expected number of additional trials to obtain HTHT is $1/(p^2q^2)$. Therefore, since in order to obtain HTHT one must first obtain HT, it follows that

$$E[\text{time to pattern HTHT}] = E[\text{time to the pattern HT}] + \frac{1}{p^2q^2}$$

To determine the expected time to the pattern HT, we can reason in the same way and let the state be the most recent 2 tosses. By the same argument as used before, it follows that the expected time between appearances of HT is equal to $1/\pi_{\text{HT}} = 1/(pq)$. As this is the same as the expected time until HT first appears, we finally obtain that

$$E[\text{time until HTHT appears}] = \frac{1}{pq} + \frac{1}{p^2q^2}$$

The same approach can be used to obtain the mean time until any given pattern appears. For instance, reasoning as before, we obtain that

$$
\begin{aligned}
E[\text{time until HTHHTHTHH}] &= E[\text{time until HTHH}] + \frac{1}{p^6q^3} \\
&= E[\text{time until H}] + \frac{1}{p^3q} + \frac{1}{p^6q^3} \\
&= \frac{1}{p} + \frac{1}{p^3q} + \frac{1}{p^6q^3}
\end{aligned}
$$

Also, it is not necessary that the basic experiment has only two possible outcomes (which we designated as H and T). For instance, if the successive values are independently and identically distributed with p_j denoting the probability that any given value is equal to j, $j \geq 0$, then

$$
\begin{aligned}
E[\text{time until } 012301] &= E[\text{time until } 01] + \frac{1}{p_0^2p_1^2p_2p_3} \\
&= \frac{1}{p_0p_1} + \frac{1}{p_0^2p_1^2p_2p_3} \qquad \blacklozenge
\end{aligned}
$$

The following result is quite useful.

Proposition 4.3 Let $\{X_n, n \geq 1\}$ be an irreducible Markov chain with stationary probabilities π_j, $j \geq 0$, and let r be a bounded function on the state space. Then, with probability 1,

$$\lim_{N\to\infty} \frac{\sum_{n=1}^{N} r(X_n)}{N} = \sum_{j=0}^{\infty} r(j)\pi_j$$

Proof If we let $a_j(N)$ be the amount of time the Markov chain spends in state j during time periods 1, ..., N, then

$$\sum_{n=1}^{N} r(X_n) = \sum_{j=0}^{\infty} a_j(N)r(j)$$

Since $a_j(N)/N \to \pi_j$ the result follows from the preceding upon dividing by N and then letting $N \to \infty$. $\blacklozenge$

If we suppose that we earn a reward $r(j)$ whenever the chain is in state j, then Proposition 4.3 states that our average reward per unit time is $\sum_j r(j)\pi_j$.

4.5. Some Applications

4.5.1. The Gambler's Ruin Problem

Consider a gambler who at each play of the game has probabilityp of winning one unit and probability q = 1 − p of losing one unit. Assuming that successive plays of the game are independent, what is the probability that, starting with i units, the gambler's fortune will reach N before reaching O?

If we let X_n denote the players fortune at time n, then the process $\{X_n, n = 0, 1, 2, \ldots\}$ is a Markov chain with transition probabilities

$$P_{00} = P_{NN} = 1,$$

$$P_{i,i+1} = p = 1 - P_{i,i-1}, \qquad i = 1, 2, \ldots, N-1$$

This Markov chain has three classes, namely, $\{0\}$, $\{1, 2, \ldots, N-1\}$, and $\{N\}$; the first and third class being recurrent and the second transient. Since each transient state is visited only finitely often, it follows that, after some finite amount of time, the gambler will either attain his goal of N or go broke.

Let P_i, $i = 0, 1, \ldots, N$, denote the probability that, starting with i, the gambler's fortune will eventually reach N. By conditioning on the outcome of the initial play of the game we obtain

$$P_i = pP_{i+1} + qP_{i-1}, \qquad i = 1, 2, \ldots, N-1$$

or equivalently, since p + q = 1,

$$pP_i + qP_i = pP_{i+1} + qP_{i-1}$$

or

$$P_{i+1} - P_i = \frac{q}{p}(P_i - P_{i-1}), \qquad i = 1, 2, \ldots, N-1$$

Hence, since $P_0 = 0$, we obtain from the preceding line that

$$P_2 - P_1 = \frac{q}{p}(P_1 - P_0) = \frac{q}{p}P_1,$$

$$P_3 - P_2 = \frac{q}{p}(P_2 - P_1) = \left(\frac{q}{p}\right)^2 P_1,$$

$$P_i - P_{i-1} = \frac{q}{p}(P_{i-1} - P_{i-2}) = \left(\frac{q}{p}\right)^{i-1} P_1,$$

$$P_N - P_{N-1} = \left(\frac{q}{p}\right)(P_{N-1} - P_{N-2}) = \left(\frac{q}{p}\right)^{N-1} P_1$$

Adding the first $i - 1$ of these equations yields

$$P_i - P_1 = P_1\left[\left(\frac{q}{p}\right) + \left(\frac{q}{p}\right)^2 + \cdots + \left(\frac{q}{p}\right)^{i-1}\right]$$

or

$$P_i = \begin{cases} \dfrac{1 - (q/p)^i}{1 - (q/p)} P_1, & \text{if } \dfrac{q}{p} \neq 1 \\ iP_1, & \text{if } \dfrac{q}{p} = 1 \end{cases}$$

Now, using the fact that $P_N = 1$, we obtain that

$$P_1 = \begin{cases} \dfrac{1 - (q/p)}{1 - (q/p)^N}, & \text{if } p \neq \dfrac{1}{2} \\ \dfrac{1}{N}, & \text{if } p = \dfrac{1}{2} \end{cases}$$

and hence

$$P_i = \begin{cases} \dfrac{1 - (q/p)^i}{1 - (q/p)^N}, & \text{if } p \neq \dfrac{1}{2} \\ \dfrac{i}{N}, & \text{if } p = \dfrac{1}{2} \end{cases} \tag{4.13}$$

Note that, as $N \to \infty$,

$$P_i \to \begin{cases} 1 - \left(\dfrac{q}{p}\right)^i, & \text{if } p > \dfrac{1}{2} \\ 0, & \text{if } p \leq \dfrac{1}{2} \end{cases}$$

Thus, if $p > \frac{1}{2}$, there is a positive probability that the gambler's fortune will increase indefinitely; while if $p \leq \frac{1}{2}$, the gambler will, with probability 1, go broke against an infinitely rich adversary.

Example 4.21 Suppose Max and Patty decide to flip pennies; the one coming closest to the wall wins. Patty, being the better player, has a probability 0.6 of winning on each flip. If Patty starts with five pennies and Max with ten, then what is the probability that Patty will wipe Max out? What if Patty starts with ten and Max with 20?

Solution: (a) The desired probability is obtained from Equation (4.13) by letting i = 5, N = 15, and p = 0.6. Hence, the desired probability is

$$\frac{1 - (\frac{2}{3})^5}{1 - (\frac{2}{3})^{15}} \approx 0.87$$

(b) The desired probability is

$$\frac{1 - (\frac{2}{3})^{10}}{1 - (\frac{2}{3})^{30}} \approx 0.98 \quad \blacklozenge$$

For an application of the gambler's ruin problem to drug testing, suppose that two new drugs have been developed for treating a certain disease. Drug i has a cure rate P_i, i = 1, 2, in the sense that each patient treated with drug i will be cured with probability P_i. These cure rates are, however, not known, and suppose we are interested in a method for deciding whether $P_1 > P_2$ or $P_2 > P_1$. To decide upon one of these alternatives, consider the following test: Pairs of patients are treated sequentially with one member of the pair receiving drug 1 and the other drug 2. The results for each pair are determined, and the testing stops when the cumulative number of cures using one of the drugs exceeds the cumulative number of cures when using the other by some fixed predetermined number. More formally, let

$$X_j = \begin{cases} 1, & \text{if the patient in the } j\text{th pair to receive drug number 1 is cured} \\ 0, & \text{otherwise} \end{cases}$$

$$Y_j = \begin{cases} 1, & \text{if the patient in the } j\text{th pair to receive drug number 2 is cured} \\ 0, & \text{otherwise} \end{cases}$$

For a predetermined positive integer M the test stops after pair N where N is the first value of n such that either

$$X_1 + \cdots + X_n - (Y_1 + \cdots + Y_n) = M$$

or

$$X_1 + \cdots + X_n - (Y_1 + \cdots + Y_n) = -M$$

In the former case we then assert that $P_1 > P_2$, and in the latter that $P_2 > P_1$.

In order to help ascertain whether the preceding is a good test, one thing we would like to know is the probability of it leading to an incorrect decision. That is, for given P_1 and P_2 where $P_1 > P_2$, what is the probability that the test will incorrectly assert that $P_2 > P_1$? To determine this probability, note that after each pair is checked the cumulative difference of cures using drug 1 versus drug 2 will either go up by 1 with probability $P_1(1 - P_2)$—since this is the probability that drug 1 leads to a cure and drug 2 does not—or go down by 1 with probability $(1 - P_1)P_2$, or remain the same with probability $P_1P_2 + (1 - P_1)(1 - P_2)$. Hence, if we only consider those pairs in which the cumulative difference changes, then the difference will go up 1 with probability

$$\begin{aligned} p &= P\{\text{up } 1 \mid \text{up } 1 \text{ or down } 1\} \\ &= \frac{P_1(1 - P_2)}{P_1(1 - P_2) + (1 - P_1)P_2} \end{aligned}$$

and down 1 with probability

$$q = 1 - p = \frac{P_2(1 - P_1)}{P_1(1 - P_2) + (1 - P_1)P_2}$$

Hence, the probability that the test will assert that $P_2 > P_1$ is equal to the probability that a gambler who wins each (one unit) bet with probability p will go down M before going up M. But Equation (4.12) with $i = M$, $N = 2M$, shows that this probability is given by

$$\begin{aligned} P\{\text{test asserts that } P_2 > P_1\} &= 1 - \frac{1 - (q/p)^M}{1 - (q/p)^{2M}} \\ &= \frac{1}{1 + (p/q)^M} \end{aligned}$$

Thus, for instance, if $P_1 = 0.6$ and $P_2 = 0.4$ then the probability of an incorrect decision is 0.017 when $M = 5$ and reduces to 0.0003 when $M = 10$.

4.5.2. A Model for Algorithmic Efficiency

The following optimization problem is called a linear program:

$$\begin{aligned} &\text{minimize } \mathbf{c}\mathbf{x}, \\ &\text{subject to } \mathbf{A}\mathbf{x} = \mathbf{b}, \\ &\mathbf{x} \geq \mathbf{0} \end{aligned}$$

where A is an $m \times n$ matrix of fixed constants; $\mathbf{c} = (c_1, \ldots, c_n)$ and $\mathbf{b} = (b_1, \ldots, b_m)$ are vectors of fixed constants, and $\mathbf{x} = (x_1, \ldots, x_n)$ is the n-vector of nonnegative values that is to be chosen to minimize $\mathbf{c}\mathbf{x} \equiv \sum_{i=1}^{n} c_i x_i$. Supposing that $n > m$, it can be shown that the optimal $\mathbf{x}$ can always be chosen to have at least $n - m$ components equal to 0—that is, it can always be taken to be one of the so-called extreme points of the feasibility region.

The simplex algorithm solves this linear program by moving from an extreme point of the feasibility region to a better (in terms of the objective function $\mathbf{cx}$) extreme point (via the pivot operation) until the optimal is reached. Because there can be as many as $N \equiv \binom{n}{m}$ such extreme points, it would seem that this method might take many iterations, but, surprisingly to some, this does not appear to be the case in practice.

To obtain a feel for whether or not the preceding statement is surprising, let us consider a simple probabilistic (Markov chain) model as to how the algorithm moves along the extreme points. Specifically, we will suppose that if at any time the algorithm is at the jth best extreme point then after the next pivot the resulting extreme point is equally likely to be any of the $j - 1$ best. Under this assumption, we show that the time to get from the Nth best to the best extreme point has approximately, for large N, a normal distribution with mean and variance equal to the logarithm (base e) of N.

Consider a Markov chain for which $P_{11} = 1$ and

$$P_{ij} = \frac{1}{i-1}, \qquad j = 1, \ldots, i-1, \; i > 1$$

and let T_i denote the number of transitions needed to go from state i to state 1. A recursive formula for $E[T_i]$ can be obtained by conditioning on the initial transition:

$$E[T_i] = 1 + \frac{1}{i-1} \sum_{j=1}^{i-1} E[T_j]$$

Starting with $E[T_1] = 0$, we successively see that

$$E[T_2] = 1,$$

$$E[T_3] = 1 + \tfrac{1}{2},$$

$$E[T_4] = 1 + \tfrac{1}{3}(1 + 1 + \tfrac{1}{2}) = 1 + \tfrac{1}{2} + \tfrac{1}{3}$$

and it is not difficult to guess and then prove inductively that

$$E[T_i] = \sum_{j=1}^{i-1} 1/j$$

However, to obtain a more complete description of T_N, we will use the representation

$$T_N = \sum_{j=1}^{N-1} I_j$$

where

$$I_j = \begin{cases} 1, & \text{if the process ever enters } j \\ 0, & \text{otherwise} \end{cases}$$

The importance of the preceding representation stems from the following:

Proposition 4.4 $I_1, \ldots, I_{N-1}$ are independent and

$$P\{I_j = 1\} = 1/j, \qquad 1 \le j \le N-1$$

Proof Given $I_{j+1}, \ldots, I_N$, let $n = \min\{i : i > j, I_i = 1\}$ denote the lowest numbered state, greater than j, that is entered. Thus we know that the process enters state n and the next state entered is one of the states $1, 2, \ldots, j$. Hence, as the next state from state n is equally likely to be any of the lower number states $1, 2, \ldots, n-1$ we see that

$$P\{I_j = 1 \mid I_{j+1}, \ldots, I_N\} = \frac{1/(n-1)}{j/(n-1)} = 1/j$$

Hence, $P\{I_j = 1\} = 1/j$, and independence follows since the preceding conditional probability does not depend on $I_{j+1}, \ldots, I_N$. ◆

Corollary 4.5

(i) $E[T_N] = \sum_{j=1}^{N-1} 1/j$.
(ii) $\text{Var}(T_N) = \sum_{j=1}^{N-1} (1/j)(1 - 1/j)$.
(iii) For N large, T_N has approximately a normal distribution with mean $\log N$ and variance $\log N$.

Proof Parts (i) and (ii) follow from Proposition 4.4 and the representation $T_N = \sum_{j=1}^{N-1} I_j$. Part (iii) follows from the central limit theorem since

$$\int_1^N \frac{dx}{x} < \sum_1^{N-1} 1/j < 1 + \int_1^{N-1} \frac{dx}{x}$$

or

$$\log N < \sum_1^{N-1} 1/j < 1 + \log(N-1)$$

and so

$$\log N \approx \sum_{j=1}^{N-1} 1/j \quad ◆$$

Returning to the simplex algorithm, if we assume that n, m, and $n - m$ are all large, we have by Stirling's approximation that

$$N = \binom{n}{m} \sim \frac{n^{n+1/2}}{(n-m)^{n-m+1/2} m^{m+1/2} \sqrt{2\pi}}$$

and so, letting $c = n/m$,

$$\log N \sim (mc + \tfrac{1}{2}) \log(mc) - (m(c-1) + \tfrac{1}{2}) \log(m(c-1)) - (m + \tfrac{1}{2}) \log m - \tfrac{1}{2} \log(2\pi)$$

or

$$\log N \sim m \left[c \log \frac{c}{c-1} + \log(c-1) \right]$$

Now, as $\lim_{x\to\infty} x \log[x/(x-1)] = 1$, it follows that, when c is large,

$$\log N \sim m[1 + \log(c-1)]$$

Thus for instance, if $n = 8000$, $m = 1000$, then the number of necessary transitions is approximately normally distributed with mean and variance equal to $1000(1 + \log 7) \approx 3000$. Hence, the number of necessary transitions would be roughly between

$$3000 \pm 2\sqrt{3000} \qquad \text{or, roughly } 3000 \pm 110,$$

95 percent of the time.

4.5.3. Using a Random Walk to Analyze a Probabilistic Algorithm for the Satisfiability Problem

Consider a Markov chain with states $0, 1, \ldots, n$ having

$$P_{0,1} = 1, \qquad P_{i,i+1} = p, \qquad P_{i,i-1} = q = 1 - p, \qquad 1 \le i \le n$$

and suppose that we are interested in studying the time that it takes for the chain to go from state 0 to state n. One approach to obtaining the mean time to reach state n would be to let m_i denote the mean time to go from state i to state n, $i = 0, \ldots, n-1$. If we then condition on the initial transition, we obtain the following set of equations:

$$\begin{aligned}
m_0 &= 1 + m_1 \\
m_i &= E[\text{time to reach } n \mid \text{next state is } i+1]p \\
&\quad + E[\text{time to reach } n \mid \text{next state is } i-1]q \\
&= (1 + m_{i+1})p + (1 + m_{i-1})q \\
&= 1 + pm_{i+1} + qm_{i-1}, \qquad i = 1, \ldots, n-1
\end{aligned}$$

Whereas the preceding equations can be solved for m_i, i = $0, \ldots,$ n $-$ 1, we do not pursue their solution; we instead make use of the special structure of the Markov chain to obtain a simpler set of equations. To start, let N_i denote the number of additional transitions that it takes the chain when it first enters state i until it enters state i + 1. By the Markovian property, it follows that these random variables N_i, i = $0, \ldots,$ n $-$ 1 are independent. Also, we can express $N_{0,n}$, the number of transitions that it takes the chain to go from state 0 to state n, as

$$N_{0,n} = \sum_{i=0}^{n-1} N_i \tag{4.14}$$

Letting $\mu_i = E[N_i]$ we obtain, upon conditioning on the next transition after the chain enters state i, that for i = 1, $\ldots,$ n $-$ 1

μ_i = 1 + E[number of additional transitions to reach i + 1 | chain to i $-$ 1]q

Now, if the chain next enters state i $-$ 1, then in order for it to reach $i + 1$ it must first return to state i and must then go from state i + 1. Hence, we have from the preceding that

$$\mu_i = 1 + E[N^*_{i-1} + N^*_i]q$$

where N^*_{i-1} and N^*_i are, respectively, the additional number of transitions to return to state i from i $-$ 1 and the number to then go from i to $i + 1$. Now, it follows from the Markovian property that these random variables have, respectively, the same distributions as N_{i-1} and N_i. In addition, they are independent (although we will only use this when we compute the variance of $N_{0,n}$). Hence, we see that

$$\text{Pi} = 1 + q(\mu_{i-1} + \text{Pi})$$

or

$$\mu_i = \frac{1}{p} + \frac{q}{p}\mu_{i-1}, \qquad i = 1, \ldots, n - 1$$

Starting with $\mu_0 = 1$, and letting $\alpha = q/p$, we obtain from the preceding recursion that

$$\mu_1 = 1/p + \text{a}$$

$$\mu_2 = 1/p + \alpha(1/p + \alpha) = 1/p + \alpha/p + \alpha^2$$

$$\mu_3 = 1/p + \alpha(1/p + \alpha/p + \alpha^2)$$

$$= 1/p + \alpha/p + \alpha^2/p + \alpha^3$$

In general, we see that

$$\mu_i = \frac{1}{p} \sum_{j=0}^{i-1} \alpha^j + \alpha^i, \qquad i = 1, \ldots, n - 1 \tag{4.15}$$

Using Equation **(4.14),** we now get

$$E[N_{0,n}] = 1 + \frac{1}{p} \sum_{i=1}^{n-1} \sum_{j=0}^{i-1} a^{r} + \sum_{i=1}^{n-1} a'$$

When p $= \frac{1}{2}$, and so a $= 1$, we see from the preceding that

$$E[N_{0,n}] = 1 + (n - 1)n + n - 1 = n^2$$

When p $\neq \frac{1}{2}$, we obtain that

$$\begin{aligned} E[N_{0,n}] &= 1 + \frac{1}{p(1 - \alpha)} \sum_{i=1}^{n-1} (1 - a') + \frac{a - a^n}{1 - \alpha} \\ &= 1 + \frac{1 + \alpha}{1 - \alpha}\left[n - 1 - \frac{(\alpha - \alpha^n)}{1 - \alpha}\right] + \frac{\alpha - \alpha^n}{1 - \alpha} \\ &= 1 + \frac{2\alpha^{n+1} - (n + 1)\alpha^2 + n - 1}{(1 - \alpha)^2} \end{aligned}$$

where the second equality used the fact that p $= 1/(1 +$ a). Therefore, we see that when a > 1, or equivalently when p $< \frac{1}{2}$, the expected number of transitions to reach n is an exponentially increasing function of n. On the other hand, when p $= \frac{1}{2}$, $E[N_{0,n}] = $ n^2, and when p $> \frac{1}{2}$, $E[N_{0,n}]$ is, for large n, essentially linear in n.

Let us now compute $\mathrm{Var}(N_{0,n})$. To do so, we will again make use of the representation given by Equation (4.14). Letting $v_i = \mathrm{Var}(N_i)$, we start by determining the v_i recursively by using the conditional variance formula. Let $S_i = 1$ if the first transition out of state i is into state i $+ 1$, and let $S_i = -1$ if the transition is into state $i - 1$, i $= 1, \ldots,$ n $- 1$. Then,

given that $S_i = 1$: $\quad N_i = 1$

giventhat&=– 1: $\quad N_i = 1 + N_{i-1}^* + N_i^*$

Hence,

$$E[N_i \mid S_i = 1] = 1$$

$$E[N_i \mid S_i = -1] = 1 + \mu_{i-1} + \mu_i$$

implying that

$$\begin{aligned}\text{Var}(E[N_i \mid S_i]) &= \text{Var}(E[N_i \mid S_i] - 1)\\ &= (\mu_{i-1} + \mu_i)^2 q - (\mu_{i-1} + \mu_i)^2 q^2\\ &= qp(\mu_{i-1} + \mu_i)^2\end{aligned}$$

Also, since N^*_{i-1} and N^*_i, the numbers of transitions to return from state $i - 1$ to i and to then go from state i to state i + 1 are, by the Markovian property, independent random variables having the same distributions as N_{i-1} and N_i, respectively, we see that

$$\text{Var}(N_i \mid S_i = 1) = 0$$

$$\text{Var}(N_i \mid S_i = -1) = v_{i-1} + v_i$$

Hence,

$$E[\text{Var}(N_i \mid S_i)] = q(v_{i-1} + v_i)$$

From the conditional variance formula, we thus obtain that

$$v_i = pq(\mu_{i-1} + \mu_i)^2 + q(v_{i-1} + v_i)$$

or, equivalently

$$v_i = q(\mu_{i-1} + \mu_i)^2 + \alpha v_{i-1} \qquad i = 1, \ldots, n - 1$$

Starting with $v_0 = 0$, we obtain from the preceding recursion that

$$\begin{aligned}v_1 &= q(\mu_0 + \mu_1)^2,\\ v_2 &= q(\mu_1 + \mu_2)^2 + \alpha q(\mu_0 + \mu_1)^2,\\ v_3 &= q(\mu_2 + \mu_3)^2 + \alpha q(\mu_1 + \mu_2)^2 + \alpha^2 q(\mu_0 + \mu_1)^2\end{aligned}$$

In general, we have for i > 0,

$$v_i = q \sum_{j=1} \alpha^{i-j}(\mu_{j-1} + \mu_j)^2 \tag{4.16}$$

Therefore, we see that

$$\text{Var}(N_{0,n}) = \sum_{i=0}^{n-1} v_i = q \sum_{i=1}^{n-1} \sum_{j=1}^{i} \alpha^{i-j}(\mu_{j-1} + \mu_j)^2$$

where μ_j is given by Equation (4.15).

We see from Equations (4.15) and (4.16) that when $p \geq \frac{1}{2}$, and so $a \leq 1$, that μ_i and v_i, the mean and variance of the number of transitions to go from state i to i + 1, do not increase too rapidly in i. For instance, when $p = \frac{1}{2}$ it follows from Equations (4.15) and (4.16) that

$$\mu_i = 2i + 1,$$

and

$$v_i = \frac{1}{2} \sum_{j=1}^{i} (4j)^2 = 8 \sum_{j=1}^{i} j^2$$

Hence, since $N_{0,n}$ is the sum of independent random variables, which are of roughly similar magnitudes when $p \geq \frac{1}{2}$, it follows in this case from the central limit theorem that $N_{0,n}$ is, for large n, approximately normally distributed. In particular, when $p = \frac{1}{2}$, $N_{0,n}$ is approximately normal with mean n^2 and variance

$$\begin{aligned}
\mathrm{Var}(N_{0,n}) &= 8 \sum_{i=1}^{n-1} \sum_{j=1}^{i} j^2 \\
&= 8 \sum_{j=1}^{n-1} \sum_{i=j}^{n-1} j^2 \\
&= 8 \sum_{j=1}^{n-1} (n-j)j^2 \\
&\approx 8 \int_1^{n-1} (n-x)x^2 \, dx \\
&\approx \tfrac{2}{3} n^4
\end{aligned}$$

Example 4.22 (The Satisfiability Problem): A Boolean variable x is one that takes on either of two values—either TRUE or FALSE. If x_i, $i \geq 1$ are Boolean variables, then a Boolean clause of the form

$$x_1 + \bar{x}_2 + x_3$$

is TRUE if x_1 is TRUE, or if x_2 is FALSE, or if x_3 is TRUE. That is, the symbol "+" means "or" and $\bar{x}$ is TRUE if x is FALSE and vice versa. A Boolean formula is a combination of clauses such as

$$(x_1 + \bar{x}_2) * (x_1 + x_3) * (x_2 + \bar{x}_3) * (\bar{x}_1 + \bar{x}_2) * (x_1 + x_2)$$

In the preceding, the terms between the parentheses represent clauses, and the formula is TRUE if all the clauses are TRUE, and is FALSE otherwise. For a given Boolean formula, the ***satisfiability problem*** is to either determine values for the variables that result in the formula being TRUE, or to determine that the formula is never true. For instance, one set of values that makes the preceding formula TRUE is to set X_1 = TRUE, x_2 = FALSE, and x_3 = FALSE.

Consider a formula of the n Boolean variables $x_1, \ldots, x_n$ and suppose that each clause in this formula refers to exactly two variables. We will now present a probabilistic algorithm that will either find values that satisfy the formula or determine to a high probability that it is not possible to satisfy it. To begin, start with an arbitrary setting of values. Then, at each stage choose a clause whose value is FALSE, and randomly choose one of the Boolean variables in that clause and change its value. That is, if the variable has value TRUE then change its value to FALSE, and vice versa. If this new setting makes the formula TRUE then stop, otherwise continue in the same fashion. If you have not stopped after $n^2(1 + 4\sqrt{\frac{2}{3}})$ repetitions, then declare that the formula cannot be satisfied. We will now argue that if there is a satisfiable assignment then this algorithm will find such an assignment with a probability very close to 1.

Let us start by assuming that there is a satisfiable assignment of truth values and let $\mathcal{A}$ be such an assignment. At each stage of the algorithm there is a certain assignment of values. Let Y_j denote the number of the n variables whose values at the jth stage of the algorithm agree with their values in $\mathcal{A}$. For instance, suppose that $n = 3$ and $\mathcal{A}$ consists of the settings $x_1 = x_2 = x_3 =$ TRUE. If the assignment of values at the jth step of the algorithm is $x_1 =$ TRUE, $x_2 = x_3 =$ FALSE, then $Y_j = 1$. Now, at each stage, the algorithm considers a clause that is not satisfied, thus implying that at least one of the values of the two variables in this clause does not agree with its value in $\mathcal{A}$. As a result, when we randomly choose one of the variables in this clause then there is a probability of at least $\frac{1}{2}$ that $Y_{j+1} = Y_j + 1$ and at most $\frac{1}{2}$ that $Y_{j+1} = Y_j - 1$. That is, independent of what has previously transpired in the algorithm, at each stage the number of settings in agreement with those in $\mathcal{A}$ will either increase or decrease by 1 and the probability of an increase is at least $\frac{1}{2}$ (it is 1 if both variables have values different from their values in $\mathcal{A}$). Thus, even though the process Y_j, $j \geq 0$ is not itself a Markov chain (why not?) it is intuitively clear that both the expectation and the variance of the number of stages of the algorithm needed to obtain the values of $\mathcal{A}$ will be less than or equal to the expectation and variance of the number of transitions to go from state 0 to state n in the Markov chain of Section 4.5.2. Hence, if the algorithm has not yet terminated because it found a set of satisfiable values different from that of $\mathcal{A}$, it will do so within an expected time of at most n^2 and with a standard deviation of at most $n^2\sqrt{\frac{2}{3}}$. In addition, since the time for the Markov chain to go from 0 to n is approximately normal when n is large we can be quite certain that a satisfiable assignment will be reached by $n^2 + 4(n^2\sqrt{\frac{2}{3}})$ stages, and thus if one has not been found by this number of stages of the algorithm we can be quite certain that there is no satisfiable assignment.

Our analysis also makes it clear why we assumed that there are only two variables in each clause. For if there were k, $k > 2$, variables in a clause then as any clause that is not presently satisfied may only have 1 incorrect setting, a randomly chosen variable whose value is changed might only increase the number of values in agreement with $\mathcal{A}$ with probability $1/k$ and so we could only conclude from our prior Markov chain results that the mean time to obtain the values in $\mathcal{A}$ is an exponential function of n, which is not an efficient algorithm when n is large. ◆

4.6. Mean Time Spent in Transient States

Consider now a finite state Markov chain and suppose that the states are numbered so that $T = \{1, 2, \ldots, t\}$ denotes the set of transient states. Let

$$\mathbf{P_T} = \begin{bmatrix} P_{11} & P_{12} & \cdots & P_{1t} \\ P_{i1} & P_{i2} & \cdots & P_{it} \\ P_{t1} & P_{t2} & \cdots & P_{tt} \end{bmatrix}$$

and note that since $\mathbf{P_T}$ specifies only the transition probabilities from transient states into transient states, some of its row sums are less than 1 (otherwise, T would be a closed class of states).

For transient states i and j, let s_{ij} denote the expected number of time periods that the Markov chain is in state j, given that it starts in state i. Let $\delta_{i,j} = 1$ when $i = j$ and let it be 0 otherwise. Condition on the initial transition to obtain

$$\begin{aligned} s_{ij} &= \delta_{i,j} + \sum_k P_{ik} s_{kj} \\ &= \delta_{i,j} + \sum_{k=1}^{t} P_{ik} s_{kj} \end{aligned} \tag{4.17}$$

where the final equality follows since it is impossible to go from a recurrent to a transient state, implying that $s_{kj} = 0$ when k is a recurrent state.

Let S denote the matrix of values s_{ij}, $i, j = 1, \ldots, t$. That is

$$\mathbf{S} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1t} \\ s_{i1} & s_{i2} & \cdots & s_{it} \\ s_{t1} & s_{t2} & \cdots & s_{tt} \end{bmatrix}$$

In matrix notation, Equation (4.17) can be written as

$$\mathbf{S} = \mathbf{I} + \mathbf{P_T S}$$

where **I** is the identity matrix of size t. Because the preceding equation is equivalent to

$$(\mathbf{I} - \mathbf{P_T})\mathbf{S} = \mathbf{I}$$

we obtain, upon multiplying both sides by $(\mathbf{I} - \mathbf{P_T})^{-1}$,

$$\mathbf{S} = (\mathbf{I} - \mathbf{P_T})^{-1}$$

That is, the quantities s_{ij}, $i \in T$, $j \in T$, can be obtained by inverting the matrix $\mathbf{1} - \mathbf{P_T}$. (The existence of the inverse is easily established.)

Example 4.23 Consider the gambler's ruin problem with $p = 0.4$ and $N = 7$. Starting with 3 units, determine

(a) the expected amount of time the gambler has 5 units,
(b) the expected amount of time the gambler has 2 units.

Solution: The matrix $\mathbf{P_T}$, which specifies P_{ij}, $i, j \in \{1, 2, 3, 4, 5, 6\}$, is as follows:

$$\mathbf{P_T} = \begin{array}{c|cccccc} & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 1 & 0 & 0.4 & 0 & 0 & 0 & 0 \\ 2 & 0.6 & 0 & 0.4 & 0 & 0 & 0 \\ 3 & 0 & 0.6 & 0 & 0.4 & 0 & 0 \\ 4 & 0 & 0 & 0.6 & 0 & 0.4 & 0 \\ 5 & 0 & 0 & 0 & 0.6 & 0 & 0.4 \\ 6 & 0 & 0 & 0 & 0 & 0.6 & 0 \end{array}$$

Inverting $\mathrm{I} - \mathbf{P_T}$ gives

$$\mathbf{S} = (\mathbf{I} - \mathbf{P_T})^{-1} = \begin{bmatrix} 1.6149 & 1.0248 & 0.6314 & 0.3691 & 0.1943 & 0.0777 \\ 1.5372 & 2.5619 & 1.5784 & 0.9228 & 0.4857 & 0.1943 \\ 1.4206 & 2.3677 & 2.9990 & 1.7533 & 0.9228 & 0.3691 \\ 1.2458 & 2.0763 & 2.6299 & 2.9990 & 1.5784 & 0.6314 \\ 0.9835 & 1.6391 & 2.0763 & 2.3677 & 2.5619 & 1.0248 \\ 0.5901 & 0.9835 & 1.2458 & 1.4206 & 1.5372 & 1.6149 \end{bmatrix}$$

Hence,

$$s_{3,5} = 0.9228, \qquad s_{3,2} = 2.3677 \quad \blacklozenge$$

For $i \in T, j \in T$, the quantity f_{ij}, equal to the probability that the Markov chain ever makes a transition into state j given that it starts in state i, is easily determined from $\mathbf{P}_T$. To determine the relationship, let us start by deriving an expression for s_{ij} by conditioning on whether state j is ever entered. This yields

$$\begin{aligned} s_{ij} &= E[\text{time in } j \mid \text{start in } i, \text{ ever transit to } j] f_{ij} \\ &\quad + E[\text{time in } j \mid \text{start in } i, \text{ never transit to } j](1 - f_{ij}) \\ &= (\delta_{i,j} + s_{jj}) f_{ij} + \delta_{i,j}(1 - f_{i,j}) \\ &= \delta_{i,j} + f_{ij} s_{jj} \end{aligned}$$

since s_{jj} is the expected number of additional time periods spent in state j given that it is eventually entered from state i. Solving the preceding equation yields

$$f_{ij} = \frac{s_{ij} - \delta_{i,j}}{s_{jj}}$$

Example 4.24 In Example 4.23, what is the probability that the gambler ever has a fortune of 1.

Solution: Since $s_{3,1} = 1.4206$ and $s_{1,1} = 1.6149$, then

$$f_{3,1} = \frac{s_{3,1}}{s_{1,1}} = 0.8797$$

As a check, note that $f_{3,1}$ is just the probability that a gambler starting with 3 reaches 1 before 7. That is, it is the probability that the gambler's fortune will go down 2 before going up 4; which is the probability that a gambler starting with 2 will go broke before reaching 6. Therefore,

$$f_{3,1} = 1 - \frac{1 - (0.6/0.4)^2}{1 - (0.6/0.4)^6} = 0.8797$$

which checks with our earlier answer. ◆

4.7. Branching Processes

In this section we consider a class of Markov chains, known as branching processes, which have a wide variety of applications in the biological, sociological, and engineering sciences.

Consider a population consisting of individuals able to produce offspring of the same kind. Suppose that each individual will, by the end of its lifetime, have produced j new offspring with probability P_j, $j \geq 0$, independently of the number produced by any other individual. We suppose that $P_j < 1$ for all $j \geq 0$. The number of individuals initially present, denoted by X_0, is called the size of the zeroth generation. All offspring of the zeroth generation constitute the first generation and their number is denoted by X_1. In general, let X_n denote the size of the nth generation. It follows that $\{X_n, n = 0, 1, \ldots\}$ is a Markov chain having as its state space the set of nonnegative integers.

Note that state 0 is a recurrent state, since clearly $P_{00} = 1$. Also, if $P_0 > 0$, all other states are transient. This follows since $P_{i0} = P_0^i$, which implies that starting with i individuals there is a positive probability of at least P_0^i that no later generation will ever consist of i individuals. Moreover, since any finite set of transient states $\{1, 2, \ldots, n\}$ will be visited only finitely often, this leads to the important conclusion that, *if* $P_0 > 0$, then the population will either die out or its size will converge to infinity.

Let

$$\mu = \sum_{j=0}^{\infty} jP_j$$

denote the mean number of offspring of a single individual, and let

$$\sigma^2 = \sum_{j=0}^{\infty} (j - \mu)^2 P_j$$

be the variance of the number of offspring produced by a single individual.

Let us suppose that $X_0 = 1$, that is, initially there is a single individual present. We calculate $E[X_n]$ and $\text{Var}(X_n)$ by first noting that we may write

$$X_n = \sum_{i=1}^{X_{n-1}} Z_i$$

where Z_i represents the number of offspring of the ith individual of the $(n - 1)$st generation. By conditioning on X_{n-1}, we obtain

$$\begin{aligned} E[X_n] &= E[E[X_n | X_{n-1}]] \\ &= E\left[E\left[\sum_{i=1}^{X_{n-1}} Z_i | X_{n-1}\right]\right] \\ &= E[X_{n-1}\mu] \\ &= \mu E[X_{n-1}] \end{aligned} \tag{4.18}$$

where we have used the fact that $E[Z_i] = \mu$. Since $E[X_0] = 1$, Equation (4.18) yields

$$
\begin{aligned}
E[X_1] &= \mu, \\
E[X_2] &= \mu E[X_1] = \mu^2, \\
&\vdots \\
E[X_n] &= \mu E[X_{n-1}] = \mu^n
\end{aligned}
$$

Similarly, $\mathrm{Var}(X_n)$ may be obtained by using the conditional variance formula

$$\mathrm{Var}(X_n) = E[\mathrm{Var}(X_n | X_{n-1})] + \mathrm{Var}(E[X_n | X_{n-1}])$$

Now, given X_{n-1}, X_n is just the sum of X_{n-1} independent random variables each having the distribution $\{P_j, j \geq 0\}$. Hence,

$$\mathrm{Var}(X_n | X_{n-1}) = X_{n-1}\sigma^2$$

Thus, the conditional variance formula yields

$$
\begin{aligned}
\mathrm{Var}(X_n) &= E[X_{n-1}\sigma^2] + \mathrm{Var}(X_{n-1}\mu) \\
&= \sigma^2\mu^{n-1} + \mu^2 \mathrm{Var}(X_{n-1})
\end{aligned}
$$

Using the fact that $\mathrm{Var}(X_0) = 0$ we can show by mathematical induction that the preceding implies

$$\mathrm{Var}(X_n) = \begin{cases} \sigma^2\mu^{n-1}\left(\dfrac{\mu^n - 1}{\mu - 1}\right), & \text{if } \mu \neq 1 \\ n\sigma^2, & \text{if } \mu = 1 \end{cases} \tag{4.19}$$

Let π_0 denote the probability that the population will eventually die out (under the assumption that $X_0 = 1$). More formally,

$$\pi_0 = \lim_{n \to \infty} P\{X_n = 0 | X_0 = 1\}$$

The problem of determining the value of π_0 was first raised in connection with the extinction of family surnames by Galton in 1889.

We first note that $\pi_0 = 1$ if $\mu < 1$. This follows since

$$
\begin{aligned}
\mu^n = E[X_n] &= \sum_{j=1}^{\infty} jP\{X_n = j\} \\
&\geq \sum_{j=1}^{\infty} 1 \cdot P\{X_n = j\} \\
&= P\{X_n \geq 1\}
\end{aligned}
$$

Since $\mu^n \to 0$ when $\mu < 1$, it follows that $P\{X_n \geq 1\} \to 0$, and hence $P\{X_n = 0\} \to 1$.

In fact, it can be shown that $\pi_0 = 1$ even when $\mu = 1$. When $\mu > 1$, it turns out that $\pi_0 < 1$, and an equation determining π_0 may be derived by conditioning on the number of offspring of the initial individual, as follows:

$$\begin{aligned}\pi_0 &= P\{\text{population dies out}\} \\ &= \sum_{j=0}^{\infty} P\{\text{population dies out} \mid X_1 = j\} P_j\end{aligned}$$

Now, given that $X_1 = j$, the population will eventually die out if and only if each of the j families started by the members of the first generation eventually dies out. Since each family is assumed to act independently, and since the probability that any particular family dies out is just π_0, this yields

$$P\{\text{population dies out} \mid X_1 = j\} = \pi_0^j$$

and thus π_0 satisfies

$$\pi_0 = \sum_{j=0}^{\infty} \pi_0^j P_j \tag{4.20}$$

In fact when $\mu > 1$, it can be shown that π_0 is the smallest positive number satisfying Equation *(4.20)*.

Example 4.25 If $P_0 = \frac{1}{2}$, $P_1 = \frac{1}{4}$, $P_2 = \frac{1}{4}$, then determine π_0.

Solution: Since $\mu = \frac{3}{4} \leq 1$, it follows that $\pi_0 = 1$. ◆

Example 4.26 If $P_0 = \frac{1}{4}$, $P_1 = \frac{1}{4}$, $P_2 = \frac{1}{2}$, then determine π_0.

Solution: π_0 satisfies

$$\pi_0 = \tfrac{1}{4} + \tfrac{1}{4}\pi_0 + \tfrac{1}{2}\pi_0^2$$

or

$$2\pi_0^2 - 3\pi_0 + 1 = 0$$

The smallest positive solution of this quadratic equation is $\pi_0 = \frac{1}{2}$. ◆

Example 4.27 In Examples *4.25* and 4.26, what is the probability that the population will die out if it initially consists of n individuals?

Solution: Since the population will die out if and only if the families of each of the members of the initial generation die out, the desired probability is π_0^n. For Example *4.25* this yields $\pi_0^n = 1$, and for Example 4.26, $\pi_0^n = (\frac{1}{2})^n$. ◆

4.8. Time Reversible Markov Chains

Consider a stationary **ergodic** Markov chain (that is, an **ergodic** Markov chain that has been in operation for a long time) having transition probabilities P_{ij} and stationary probabilities π_i, and suppose that starting at some time we trace the sequence of states going backwards in time. That is, starting at time n, consider the sequence of states $X_n, X_{n-1}, X_{n-2}, \ldots$. It turns out that this sequence of states is itself a Markov chain with transition probabilities Q_{ij} defined by

$$\begin{aligned} Q_{ij} &= P\{X_m = j \mid X_{m+1} = i\} \\ &= \frac{P\{X_m = j, X_{m+1} = i\}}{P\{X_{m+1} = i\}} \\ &= \frac{P\{X_m = j\}P\{X_{m+1} = i \mid X_m = j\}}{P\{X_{m+1} = i\}} \\ &= \frac{\pi_j P_{ji}}{\pi_i} \end{aligned}$$

To prove that the reversed process is indeed a Markov chain, we must verify that

$$P\{X_m = j \mid X_{m+1} = i, X_{m+2}, X_{m+3}, \ldots\} = P\{X_m = j \mid X_{m+1} = i\}$$

To see that this is so, suppose that the present time is m + 1. Now, since $X_0, X_1, X_2, \ldots$ is a Markov chain, it follows that the conditional distribution of the future $X_{m+2}, X_{m+3}, \ldots$ given the present state X_{m+1} is independent of the past state X_m. However, independence is a symmetric relationship (that is, if A is independent of B, then B is independent of A), and so this means that given X_{m+1}, X_m is independent of $X_{m+2}, X_{m+3}, \ldots$. But this is exactly what we had to verify.

Thus, the reversed process is also a Markov chain with transition probabilities given by

$$Q_{ij} = \frac{\pi_j P_{ji}}{\pi_i}$$

If $Q_{ij} = P_{ij}$ for all i, j, then the Markov chain is said to be time reversible. The condition for time reversibility, namely, $Q_{ij} = P_{ij}$, can also be expressed as

$$\pi_i P_{ij} = \pi_j P_{ji} \qquad \text{for all } i, j \tag{4.21}$$

The condition in Equation (4.21) can be stated that, for all states i and j, the rate at which the process goes from i to j (namely, $\pi_i P_{ij}$) is equal to the rate at which it goes from j to i (namely, $\pi_j P_{ji}$). It is worth noting that this is an obvious necessary condition for time reversibility since a transition from i to j going backward in time is equivalent to a transition from j to i going forward in time; i.e., if $X_m = i$ and $X_{m-1} = j$, then a transition from i to j is observed if we are looking backward, and one from j to i if we are looking forward in time. Thus, the rate at which the forward process makes a transition from j to i is always equal to the rate at which the reverse process makes a transition from i to j; if time reversible, this must equal the rate at which the forward process makes a transition from i to j.

If we can find nonnegative numbers, summing to one, which satisfy Equation (4.21), then it follows that the Markov chain is time reversible and the numbers represent the limiting probabilities. This is so since if

$$x_i P_{ij} = x_j P_{ji} \qquad \text{for all } i, j, \ \sum_i x_i = 1 \tag{4.22}$$

Then summing over i yields

$$\sum_i x_i P_{ij} = x_j \sum_i P_{ji} = x_j, \qquad \sum_i x_i = 1$$

and, as the limiting probabilities π_i are the unique solution of the above, it follows that $x_i = \pi_i$ for all i.

Example 4.28 Consider a random walk with states $0, 1, \ldots, M$ and transition probabilities

$$\begin{aligned} P_{i,i+1} &= \alpha_i = 1 - P_{i,i-1}, \qquad i = 1, \ldots, M-1, \\ P_{0,1} &= \alpha_0 = 1 - P_{0,0}, \\ P_{M,M} &= \alpha_M = 1 - P_{M,M-1} \end{aligned}$$

Without the need of any computations, it is possible to argue that this Markov chain, which can only make transitions from a state to one of its two nearest neighbors, is time reversible. This follows by noting that the number of transitions from i to $i + 1$ must at all times be within 1 of the number from $i + 1$ to i. This is so since between any two transitions from i to $i + 1$ there must be one from $i + 1$ to i (and conversely) since the only way to reenter i from a higher state is via state $i + 1$. Hence, it follows that the rate of transitions from i to $i + 1$ equals the rate from $i + 1$ to i, and so the process is time reversible.

We can easily obtain the limiting probabilities by equating for each state $i = 0, 1, \ldots, M - 1$ the rate at which the process goes from i to $i + 1$ with the.rate at which it goes from i + 1 to i. This yields

$$\pi_0\alpha_0 = \pi_1(1 - \alpha_1),$$
$$\pi_1\alpha_1 = \pi_2(1 - \alpha_2),$$
$$\vdots$$
$$\pi_i\alpha_i = \pi_{i+1}(1 - \alpha_{i+1}), \qquad i = 0, 1, \ldots, M - 1$$

Solving in terms of π_0 yields

$$\pi_1 = \frac{\alpha_0}{1 - \alpha_1}\pi_0,$$

$$\pi_2 = \frac{\alpha_1}{1 - \alpha_2}\pi_1 = \frac{\alpha_1\alpha_0}{(1 - \alpha_2)(1 - \alpha_1)}\pi_0$$

and, in general,

$$\pi_i = \frac{\alpha_{i-1}\cdots\alpha_0}{(1 - \alpha_i)\cdots(1 - \alpha_1)}\pi_0, \qquad i = 1, 2, \ldots, M$$

Since $\sum_0^M \pi_i = 1$, we obtain

$$\pi_0\left[1 + \sum_{j=1}^{M} \frac{\alpha_{j-1}\cdots\alpha_0}{(1 - \alpha_j)\cdots(1 - \alpha_1)}\right] = 1$$

or

$$\pi_0 = \left[1 + \sum_{j=1}^{M} \frac{\alpha_{j-1}\cdots\alpha_0}{(1 - \alpha_j)\cdots(1 - \alpha_1)}\right]^{-1} \tag{4.23}$$

and

$$\pi_i = \frac{\alpha_{i-1}\cdots\alpha_0}{(1 - \alpha_i)\cdots(1 - \alpha_1)}\pi_0, \qquad i = 1, \ldots, M \tag{4.24}$$

For instance, if $\alpha_i \equiv \alpha$, then

$$\pi_0 = \left[1 + \sum_{j=1}^{M}\left(\frac{\alpha}{1 - \alpha}\right)^j\right]^{-1}$$
$$= \frac{1 - \beta}{1 - \beta^{M+1}}$$

and, in general,

$$\pi_i = \frac{\beta^i(1 - \beta)}{1 - \beta^{M+1}}, \qquad i = 0, 1, \ldots, M$$

where

$$\beta = \frac{\alpha}{1 - \alpha} \quad \blacklozenge$$

Another special case of Example 4.28 is the following urn model, proposed by the physicists P. and T. Ehrenfest to describe the movements of molecules. Suppose that M molecules are distributed among two urns; and at each time point one of the molecules is chosen at random, removed from its urn, and placed in the other one. The number of molecules in urn I is a special case of the Markov chain of Example 4.28 having

$$\alpha_i = \frac{M - i}{M}, \qquad i = 0, 1, \ldots, M$$

Hence, using Equations (4.23) and (4.24) the limiting probabilities in this case are

$$\begin{aligned}\pi_0 &= \left[1 + \sum_{j=1}^{M} \frac{(M - j + 1)\cdots(M - 1)M}{j(j - 1)\cdots 1}\right]^{-1} \\ &= \left[\sum_{j=0}^{M} \binom{M}{j}\right]^{-1} \\ &= \left(\frac{1}{2}\right)^{M}\end{aligned}$$

where we have used the identity

$$\begin{aligned}1 &= \left(\frac{1}{2} + \frac{1}{2}\right)^{M} \\ &= \sum_{j=0}^{M} \binom{M}{j}\left(\frac{1}{2}\right)^{M}\end{aligned}$$

Hence, from Equation (4.24)

$$\pi_i = \binom{M}{i}\left(\frac{1}{2}\right)^{M}, \qquad i = 0, 1, \ldots, M$$

As the preceding are just the binomial probabilities, it follows that in the long run, the positions of each of the M balls are independent and each one is equally likely to be in either urn. This, however, is quite intuitive, for if we focus on any one ball, it becomes quite clear that its position will be independent of the positions of the other balls (since no matter where the other $M - 1$ balls are, the ball under consideration at each stage will be moved with probability $1/M$) and by symmetry, it is equally likely to be in either urn.

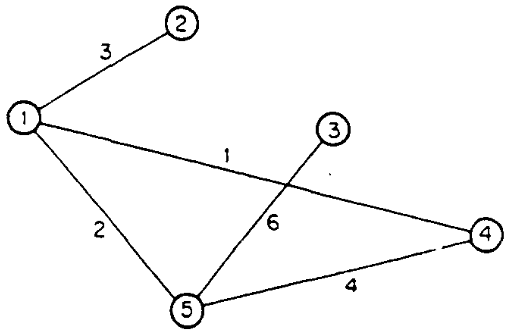

Figure 4.1. A connected graph with arc weights.

Example 4.29 Consider an arbitrary connected graph (see Section 3.6 for definitions) having a number w_{ij} associated with arc (i, j) for each arc. One instance of such a graph is given by Figure 4.1. Now consider a particle moving from node to node in this manner: If at any time the particle resides at node i, then it will next move to node j with probability P_{ij} where

$$P_{ij} = \frac{w_{ij}}{\sum_j w_{ij}}$$

and where w_{ij} is 0 if (i, j) is not an arc. For instance, for the graph of Figure 4.1, $P_{12} = 3/(3 + 1 + 2) = \frac{1}{2}$.

The time reversibility equations

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

reduce to

$$\pi_i \frac{w_{ij}}{\sum_j w_{ij}} = \pi_j \frac{w_{ji}}{\sum_i w_{ji}}$$

or, equivalently, since $w_{ij} = w_{ji}$

$$\frac{\pi_i}{\sum_j w_{ij}} = \frac{\pi_j}{\sum_i w_{ji}}$$

which is equivalent to

$$\frac{\pi_i}{\sum_j w_{ij}} = c$$

or

$$\pi_i = c \sum_j w_{ij}$$

or, since $1 = \sum_i \pi_i$

$$\pi_i = \frac{\sum_j w_{ij}}{\sum_i \sum_j w_{ij}}$$

As the π_i's given by this equation satisfy the time reversibility equations, it follows that the process is time reversible with these limiting probabilities.

For the graph of Figure 4.1 we have that

$\pi_1 = \frac{6}{32}$, $\pi_2 = \frac{3}{32}$, 7r3 = fir, $\pi_4 = \frac{5}{32}$, $\pi_5 = \frac{12}{32}$ ◆

If we try to solve Equation (4.22) for an arbitrary Markov chain with states $0, 1, \ldots, M$, it will usually turn out that no solution exists. For example, from Equation **(4.22),**

$$x_i P_{ij} = x_j P_{ji},$$

$$x_k P_{kj} = x_j P_{jk}$$

implying (if $P_{ij}P_{jk} > 0$) that

$$\frac{x_i}{x_k} = \frac{P_{ji}P_{kj}}{P_{ij}P_{jk}}$$

which in general need not equal P_{ki}/P_{ik}. Thus, we see that a necessary condition for time reversibility is that

$$P_{ik}P_{kj}P_{ji} = P_{ij}P_{jk}P_{ki} \qquad \text{for all } i, j, k \tag{4.25}$$

which is equivalent to the statement that, starting in state i, the path $i \to k \to j \to i$ has the same probability as the reversed path $i \to j \to k \to i$. To understand the necessity of this note that time reversibility implies that the rate at which a sequence of transitions from i to k to j to i occurs must equal the rate of ones from i to j to k to i (why?), and so we must have

$$\pi_i P_{ik}P_{kj}P_{ji} = \pi_i P_{ij}P_{jk}P_{ki}$$

implying Equation (4.25) when $\pi_i > 0$.

In fact, we can show the following:

Theorem 4.2 An **ergodic** Markov chain for which $P_{ij} = 0$ whenever $P_{ji} = 0$ is time reversible if and only if starting in state i, any path back to i has the same probability as the reversed path. That is, if

$$P_{i,i_1}P_{i_1,i_2}\cdots P_{i_k,i} = P_{i,i_k}P_{i_k,i_{k-1}}\cdots P_{i_1,i} \tag{4.26}$$

for all states $i, i_1, \ldots, i_k$.

Proof We have already proven necessity. To prove sufficiency, fix states i and j and rewrite (4.26) as

$$P_{i,i_1}P_{i_1,i_2}\cdots P_{i_k,j}P_{ji} = P_{ij}P_{j,i_k}\cdots P_{i_1,i}$$

Summing the above over all states $i_1, \ldots, i_k$ yields

$$P_{ij}^{k+1}P_{ji} = P_{ij}P_{ji}^{k+1}$$

Letting $k \to \infty$ yields

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

which proves the theorem. ◆

Example 4.30 Suppose we are given a set of n elements, numbered 1 through n, which are to be arranged in some ordered list. At each unit of time a request is made to retrieve one of these elements, element i being requested (independently of the past) with probability P_i. After being requested, the element then is put back but not necessarily in the same position. In fact, let us suppose that the element requested is moved one closer to the front of the list; for instance, if the present list ordering is 1, 3, 4, 2, 5 and element 2 is requested, then the new ordering becomes 1, 3, 2, 4, 5. We are interested in the long-run average position of the element requested.

For any given probability vector $\mathbf{P} = (P_1, \ldots, P_n)$, the preceding can be modeled as a Markov chain with n! states, with the state at any time being the list order at that time. We shall show that this Markov chain is time reversible and then use this to show that the average position of the element requested when this one-closer rule is in effect is less than when the rule of always moving the requested element to the front of the line is used. The time reversibility of the resulting Markov chain when the one-closer reordering rule is in effect easily follows from Theorem 4.2. For instance, suppose $n = 3$ and consider the following path from state (1, 2, 3) to itself

$$(1, 2, 3) \to (2, 1, 3) \to (2, 3, 1) \to (3, 2, 1) \to (3, 1, 2) \to (1, 3, 2) \to (1, 2, 3)$$

The product of the transition probabilities in the forward direction is

$$P_2P_3P_3P_1P_1P_2 = P_1^2P_2^2P_3^2$$

whereas in the reverse direction, it is

$$P_3P_3P_2P_2P_1P_1 = P_1^2P_2^2P_3^2$$

As the general result follows in much the same manner, the Markov chain is indeed time reversible. (For a formal argument note that if f_i denotes the number of times element i moves forward in the path, then as the path goes from a fixed state back to itself, it follows that element i will also move backwards f_i times. Therefore, since the backwards moves of element i are precisely the times that it moves forward in the reverse path, it follows that the product of the transition probabilities for both the path and its reversal will equal

$$\prod_i P_i^{f_i + r_i}$$

where r_i is equal to the number of times that element i is in the first position and the path (or the reverse path) does not change states.)

For any permutation $i_1, i_2, \dots, i_n$ of $1, 2, \dots, n$, let $\pi(i_1, i_2, \dots, i_n)$ denote the limiting probability under the one-closer rule. By time reversibility we have

$$P_{i_{j+1}} \pi(i_1, \dots, i_j, i_{j+1}, \dots, i_n) = P\ \pi(i_1, \dots, i_{j+}, \ , \ \dots, i_n) \tag{4.27}$$

for all permutations.

Now the average position of the element requested can be expressed (as in Section **3.6.1**) as

$$\text{Average position} = \sum_i P_i E[\text{Position of element i}]$$

$$= \sum_i P_i \left[1 + \sum_{j \neq i} P\{\text{element j precedes element i}\} \right]$$

$$= 1 + \sum_i \sum_{j \neq i} P_i P\{e_j \text{ precedes } e_i\}$$

$$= 1 + \sum_{i<j} [P_i P\{e_j \text{ precedes } e_i\} + P_j P\{e_i \text{ precedes } e_j\}]$$

$$= 1 + \sum_{i<j} [P_i P\{e_j \text{ precedes } e_i\} + P_j(1 - P\{e_j \text{ precedes } e_i\})]$$

$$= 1 + \sum_{i<j}\sum (P_i - P_j) P\{e_j \text{ precedes } e_i\} + \sum_{icj}\sum P_j$$

Hence, to minimize the average position of the element requested, we would want to make $P\{e_j \text{ precedes } e_i\}$ as large as possible when $P_j > P_i$ and as small as possible when $P_i > P_j$. Now under the front-of-the-line rule we showed in Section **3.6.1** that

$$P\{e_j \text{ precedes } e_i\} = \frac{P_j}{P_j + P_i}$$

(since under the front-of-the-line rule element j will precede element i if and only if the last request for either i or j was for j).

Therefore, to show that the one-closer rule is better than the front-of-the-line rule, it suffices to show that under the one-closer rule

$$P\{e_j \text{ precedes } e_i\} > \frac{P_j}{P_j + P_i} \qquad \text{when } P_j > P_i$$

Now consider any state where element i precedes element j, say $(\ldots, i, i_1, \ldots, i_k, j, \ldots)$. By successive transpositions using Equation (4.27), we have

$$\pi(\ldots, i, i_1, \ldots, i_k, j, \ldots) = \left(\frac{P_i}{P_j}\right)^{k+1} \pi(\ldots, j, i_1, \ldots, i_k, i, \ldots) \quad (4.28)$$

For instance,

$$\begin{aligned}\pi(1, 2, 3) &= \frac{P_2}{P_3}\pi(1, 3, 2) = \frac{P_2}{P_3}\frac{P_1}{P_3}\pi(3, 1, 2) \\ &= \frac{P_2}{P_3}\frac{P_1}{P_3}\frac{P_1}{P_2}\pi(3, 2, 1) = \left(\frac{P_1}{P_3}\right)^2 \pi(3, 2, 1)\end{aligned}$$

Now when $P_j > P_i$, Equation (4.28) implies that

$$\pi(\ldots, i, i_1, \ldots, i_k, j, \ldots) < \frac{P_i}{P_j}\pi(\ldots, j, i_1, \ldots, i_k, i, \ldots)$$

Letting $\alpha(i, j) = P\{e_i \text{ precedes } e_j\}$, we see by summing over all states for which i precedes j and by using the preceding that

$$\alpha(i, j) < \frac{P_i}{P_j}\alpha(j, i)$$

which, since $\alpha(i, j) = 1 - \alpha(j, i)$, yields

$$\alpha(j, i) > \frac{P_j}{P_j + P_i}$$

Hence, the average position of the element requested is indeed smaller under the one-closer rule than under the front-of-the-line rule. ◆

The concept of the reversed chain is useful even when the process is not time reversible. To illustrate this, we start with the following proposition whose proof is left as an exercise.

Proposition 4.6 Consider an irreducible Markov chain with transition probabilities P_{ij}. If one can find positive numbers π_i, $i \geq 0$, summing to one, and a transition probability matrix $Q = [Q_{ij}]$ such that

$$\pi_i P_{ij} = \pi_j Q_{ji} \tag{4.29}$$

then the Q_{ij} are the transition probabilities of the reversed chain and the π_i are the stationary probabilities both for the original and reversed chain.

The importance of the preceding proposition is that, by thinking backwards, we can sometimes guess at the nature of the reversed chain and then use the set of equations (4.29) to obtain both the stationary probabilities and the Q_{ij}.

Example 4.31 A single bulb is necessary to light a given room. When the bulb in use fails, it is replaced by a new one at the beginning of the next day. Let X_n equal i if the bulb in use at the beginning of day n is in its ith day of use (that is, if its present age is i). For instance, if a bulb fails on day $n - 1$, then a new bulb will be put in use at the beginning of day n and so $X_n = 1$. If we suppose that each bulb, independently, fails on its ith day of use with probability p_i, $i \geq 1$, then it is easy to see that $\{X_n, n \geq 1)$ is a Markov chain whose transition probabilities are as follows:

$$\begin{aligned} P_{i,1} &= P\{\text{bulb, on its ith day of use, fails}) \\ &= P\{\text{life of bulb} = i \mid \text{life of bulb} \geq i\} \\ &= \frac{P\{L = i\}}{P\{L \geq i\}} \end{aligned}$$

where L, a random variable representing the lifetime of a bulb, is such that $P[L = i\} = p_i$. Also,

$$P_{i,i+1} = 1 - P_{i,1}$$

Suppose now that this chain has been in operation for a long (in theory, an infinite) time and consider the sequence of states going backwards in time. Since, in the forward direction, the state is always increasing by 1 until it reaches the age at which the item fails, it is easy to see that the reverse chain will always decrease by 1 until it reaches 1 and then it will jump to a random value representing the lifetime of the (in real time) previous bulb. Thus, it seems that the reverse chain should have transition probabilities given by

$$\begin{aligned} Q_{i,i-1} &= 1, \qquad i > 1 \\ Q_{1,i} &= p_i, \qquad i \geq 1 \end{aligned}$$

To check this, and at the same time determine the stationary probabilities, we must see if we can find, with the $Q_{i,j}$ as given above, positive numbers $\{\pi_i\}$

such that

$$\pi_i P_{i,j} = \pi_j Q_{j,i}$$

To begin, let $j = 1$ and consider the resulting equations:

$$\pi_i P_{i,1} = \pi_1 Q_{1,i}$$

This is equivalent to

$$\pi_i \frac{P\{L = i\}}{P\{L \geq i\}} = \pi_1 P\{L = i\}$$

or

$$\pi_i = \pi_1 P\{L \geq i\}$$

Summing over all i yields

$$1 = \sum_{i=1}^{\infty} \pi_i = \pi_1 \sum_{i=1}^{\infty} P\{L \geq i\} = \pi_1 E[L]$$

and so, for the Q_{ij} above to represent the reverse transition probabilities, it is necessary that the stationary probabilities are

$$\pi_i = \frac{P\{L \geq i\}}{E[L]}, \qquad i \geq 1$$

To finish the proof that the reverse transition probabilities and stationary probabilities are as given all that remains is to show that they satisfy

$$\pi_i P_{i,i+1} = \pi_{i+1} Q_{i+1,i}$$

which is equivalent to

$$\frac{P\{L \geq i\}}{E[L]}\left(1 - \frac{P\{L = i\}}{P\{L \geq i\}}\right) = \frac{P\{L \geq i + 1\}}{E[L]}$$

and which is true since $P\{L \geq i\} - P\{L = i\} = P\{L \geq i + 1\}$. ◆

4.9. Markov Chain Monte Carlo Methods

Let X be a discrete random vector whose set of possible values is $\mathbf{x}_j$, $j \geq 1$. Let the probability mass function of X be given by $P\{X = \mathbf{x}_j\}$, $j \geq 1$, and suppose that we are interested in calculating

$$\theta = E[h(\mathbf{X})] = \sum_{j=1}^{\infty} h(\mathbf{x}_j) P\{\mathbf{X} = \mathbf{x}_j\}$$

for some specified function h. In situations where it is computationally difficult to evaluate the function $h(\mathbf{x}_j)$, $j \geq 1$, we often turn to simulation to approximate θ. The usual approach, called Monte *Carlo* simulation, is to use random numbers to generate a partial sequence of independent and identically distributed random vectors $\mathbf{X}_1, \mathbf{X}_2, \ldots,$ X, having the mass function P(X = $\mathbf{x}_j$}, j ≥ 1 (see Chapter 11 for a discussion as to how this can be accomplished). Since the strong law of large numbers yields

$$\lim_{n\to\infty} \sum_{i=1}^{n} \frac{h(\mathbf{X}_i)}{n} - 8 \tag{4.30}$$

it follows that we can estimate 6 by letting n be large and using the average of the values of $h(\mathbf{X}_i)$, i = 1, ..., n as the estimator.

It often, however, turns out that it is difficult to generate a random vector having the specified probability mass function, particularly if X is a vector of dependent random variables. In addition, its probability mass function is sometimes given in the form $P\{\mathbf{X} = \mathbf{x}_j\} = Cb_j$, j ≥ 1, where the b_j are specified, but C must be computed, and in many applications it is not computationally feasible to sum the b_j so as to determine C. Fortunately, however, there is another way of using simulation to estimate θ in these situations. It works by generating a sequence, not of independent random vectors, but of the successive states of a vector-valued Markov chain $\mathbf{X}_1, \mathbf{X}_2, \ldots$ whose stationary probabilities are $P\{\mathbf{X} = \mathbf{x}_j\}$, $j \geq 1$. If this can be accomplished, then it would follow from Proposition **4.3** that Equation **(4.30)** remains valid, implying that we can then use $\sum_{i=1}^{n} h(\mathbf{X}_i)/n$ as an estimator of θ.

We now show how to generate a Markov chain with arbitrary stationary probabilities that may only be specified up to a multiplicative constant. Let $b(j)$, $j = 1, \ldots$ be positive numbers whose sum B = $\sum_{j=1}^{\infty} b(j)$ is finite. The following, known as the Hastings–Metropolis algorithm, can be used to generate a time reversible Markov chain whose stationary probabilities are

$$\pi(j) = b(j)/B, \qquad j = 1, \ldots$$

To begin, let Q be any specified irreducible Markov transition probability matrix on the integers, with $q(i, j)$ representing the row i column j element of **Q.** Now define a Markov chain $\{X_n, n \geq 0\}$ as follows. When $X_n = i$, generate a random variable Y such that $P(Y = j) = q(i, j)$, $j = 1, \ldots$. If Y = j, then set X_{n+1} equal to j with probability $\alpha(i, j)$, and set it equal to i with probability $1 - \alpha(i, j)$. Under these conditions, it is easy to see that the sequence of states constitutes a Markov chain with transition probabilities $P_{i,j}$ given by

$$P_{i,j} = q(i,j)\alpha(i,j), \qquad \text{if } j \neq i$$

$$P_{i,i} = q(i,i) + \sum_{k \neq i} q(i,k)(1 - \alpha(i,k))$$

This Markov chain will be time reversible and have stationary probabilities $\pi(j)$ if

$$\pi(i)P_{i,j} = \pi(j)P_{j,i} \qquad \text{for } j \neq i$$

which is equivalent to

$$\pi(i)q(i,j)\alpha(i,j) = \pi(j)q(j,i)\alpha(j,i) \tag{4.31}$$

But if we take $\pi_j = b(j)/B$ and set

$$\alpha(i,j) = \min\left(\frac{\pi(j)q(j,i)}{\pi(i)q(i,j)}, 1\right) \tag{4.32}$$

then Equation (4.31) is easily seen to be satisfied. For if

$$\alpha(i,j) = \frac{\pi(j)q(j,i)}{\pi(i)q(i,j)}$$

then $\alpha(j,i) = 1$ and Equation (4.31) follows, and if $\alpha(i,j) = 1$ then

$$\alpha(j,i) = \frac{\pi(i)q(i,j)}{\pi(j)q(j,i)}$$

and again Equation (4.31) holds, thus showing that the Markov chain is time reversible with stationary probabilities $\pi(j)$. Also, since $\pi(j) = b(j)/B$, we see from (4.32) that

$$\alpha(i,j) = \min\left(\frac{b(j)q(j,i)}{b(i)q(i,j)}, 1\right)$$

which shows that the value of B is not needed to define the Markov chain, because the values $b(j)$ suffice. Also, it is almost always the case that $\pi(j)$, $j \geq 1$ will not only be stationary probabilities but will also be limiting probabilities. (Indeed, a sufficient condition is that $P_{i,i} > 0$ for some i.)

Example 4.32 Suppose that we want to generate a uniformly distributed element in S, the set of all permutations $(x_1, \ldots, x_n)$ of the numbers $(1, \ldots, n)$ for which $\sum_{j=1}^{n} jx_j > a$ for a given constant a. To utilize the Hastings–Metropolis algorithm we need to define an irreducible Markov transition probability matrix on the state space S. To accomplish this, we first define a concept of "neighboring" elements of S, and then construct a graph whose vertex set is S. We start by putting an arc between each pair of neighboring elements in S, where any two permutations in S are said to be neighbors if one results from an interchange of two of the positions of the other. That is, $(1,2,3,4)$ and $(1,2,4,3)$ are neighbors whereas $(1,2,3,4)$ and $(1,3,4,2)$ are not. Now, define the q transition probability function as follows. With $N(\mathbf{s})$ defined as the set of neighbors of s, and $|N(\mathbf{s})|$ equal to the number of elements in the set $N(\mathbf{s})$, let

$$q(\mathbf{s}, \mathbf{t}) = \frac{1}{|N(\mathbf{s})|} \qquad \text{if } \mathbf{t} \in N(\mathbf{s})$$

That is, the candidate next state from $\mathbf{s}$ is equally likely to be any of its neighbors. Since the desired limiting probabilities of the Markov chain are $\pi(\mathbf{s}) = C$, it follows that $\pi(\mathbf{s}) = \pi(\mathbf{t})$, and so

$$\alpha(\mathbf{s}, \mathbf{t}) = \min(|N(\mathbf{s})|/|N(\mathbf{t})|, 1)$$

That is, if the present state of the Markov chain is s then one of its neighbors is randomly chosen, say, t. If t is a state with fewer neighbors than s (in graph theory language, if the degree of vertex t is less than that of vertex s), then the next state is t. If not, a uniform (0, 1) random number U is generated and the next state if t if $U < |N(\mathbf{s})|/|N(\mathbf{t})|$ and is s otherwise. The limiting probabilities of this Markov chain are $\pi(\mathbf{s}) = 1/|\mathcal{S}|$, where $|\mathcal{S}|$ is the (unknown) number of permutations in S.

The preceding does not specify how to randomly choose a neighbor permutation of s. One possibility, which is efficient when n is small enough so that we can easily keep track of all the neighbors of s, is to just randomly choose one, call it t, as the target next state. The number of the neighbors of t would then have to be determined, and the next state of the Markov chain would then either be t with probability $\min(1, |N(\mathbf{s})|/|N(\mathbf{t})|)$ or it would remain s otherwise. However, if n is large this may be impractical, and a better approach might be to expand the state space to consist of all n! permutations. The desired limiting probability mass function is then

$$\pi(\mathbf{s}) = \begin{cases} C, & \mathbf{s} \in \mathcal{S} \\ 0, & \mathbf{s} \notin \mathcal{S} \end{cases}$$

With this setup, each permutation s has $\binom{n}{2}$ neighbors, and one can be randomly chosen by generating a random subset of size two from the set $1, \ldots, n$ and if i and j are chosen then the candidate next state t is obtained by interchanging the values of the ith and jth coordinates of s. If $\mathbf{t} \in \mathcal{S}$ then t becomes the next state of the chain, and if not then the next state remains s. ◆

The most widely used version of the Hastings–Metropolis algorithm is the Gibbs sampler. Let $\mathbf{X} = (X_1, \ldots, X_n)$ be a random vector with probability mass function $p(\mathbf{x})$, which may only be specified up to a multiplicative constant, and suppose that we want to generate a random vector whose distribution is that of the conditional distribution of X given that $X \in \mathcal{A}$ for some set $\mathcal{A}$. That is, we want to generate a random vector having mass function

$$f(\mathbf{x}) = \frac{p(\mathbf{x})}{P\{\mathbf{X} \in \mathcal{A}\}} \qquad \text{for } \mathbf{x} \in \mathcal{A}$$

The Gibbs sampler assumes that for any i, $i = 1, \dots, n$ and values $x_j, j \neq i$, we can generate a random variable X having the probability mass function

$$P\{X = x\} = P\{X_i = x \mid X_j = x_j, j \neq i\}$$

It operates by considering a Markov chain with states

$$\mathbf{x} = (x_1, \dots, x_i, \dots, x_n) \in \mathcal{A}$$

and then uses the Hastings–Metropolis algorithm with Markov transition probabilities defined as follows. Whenever the present state is x, a coordinate that is equally likely to be any of $1, \dots, n$ is generated. If coordinate i is the one chosen, then a random variable X having probability mass function $P\{X = x\} = P\{X_i = x \mid X_j = x_j, j \neq i\}$ is generated, and if $X = x$ then the state $y = (x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_n)$ is considered as a candidate for transition. In other words, the Gibbs sampler uses the Hastings–Metropolis algorithm with

$$q(\mathbf{x}, \mathbf{y}) = \frac{1}{n} P\{X_i = x \mid X_j = x_j, j \neq i\} = \frac{1}{n} \frac{p(\mathbf{y})}{P\{X_j = x_j, j \neq i\}}$$

Since we want the limiting mass function to be f, we have from Equation (4.32) that the vector y is then accepted as the new state with probability

$$\alpha(\mathbf{x}, \mathbf{y}) = \min\left(\frac{f(\mathbf{y})q(\mathbf{y}, \mathbf{x})}{f(\mathbf{x})q(\mathbf{x}, \mathbf{y})}, 1\right)$$

Now, for $\mathbf{x} \in \mathcal{A}$ and $y \in \mathcal{A}$

$$\frac{f(\mathbf{y})q(\mathbf{y}, \mathbf{x})}{f(\mathbf{x})q(\mathbf{x}, \mathbf{y})} = \frac{f(\mathbf{y})p(\mathbf{x})}{f(\mathbf{x})p(\mathbf{y})} = 1$$

whereas for $\mathbf{x} \in \mathcal{A}$ and $y \notin \mathcal{A}$ we have [since $f(\mathbf{y}) = 0$]

$$\frac{f(\mathbf{y})q(\mathbf{y}, \mathbf{x})}{f(\mathbf{x})q(\mathbf{x}, \mathbf{y})} = 0$$

Hence, the next state is either y if $y \in \mathcal{A}$ or it remains $\mathbf{x}$ if $y \notin \mathcal{A}$.

Example 4.33 Suppose we want to generate n uniformly distributed points in the circle of radius 1 centered at the origin, conditional on the event that no two points are within a distance d of each other, where

$$\beta = P\{\text{no two points are within d of each other})$$

is assumed to be a small positive number. (If β were not small, then we could just continue to generate sets of n uniformly distributed points in the circle, stopping the first time that no two points in the set are within d of each other.) This can be accomplished by the Gibbs sampler by starting with any n points in the circle, $\mathbf{x}_1, \ldots, \mathbf{x}_n$, for which no two are within a distance d of each other. Then generate the value of a random variable $\mathbf{I}$ that is equally likely to be any of the values $1, \ldots, n$. Also generate a random point in the circle (see Chapter 11 for details of these generations). If this point is not within d of any of the other $n - 1$ points excluding $\mathbf{x}_I$ then replace $\mathbf{x}_I$ by this generated point, otherwise do not make a change. After a large number of iterations the set of n points will approximately have the desired distribution. ◆

The Gibbs sampler for generating a random vector X conditional on the event that $X \in \mathcal{A}$ moves from state to state by choosing a coordinate $\mathbf{I}$ at random and then generating a random variable from the conditional distribution of X_I given the values of the other random variables, $X_j, j \neq \mathbf{I}$. If the vector obtained by replacing the old value of X_I by this generated value remains in $\mathcal{A}$ then it becomes the next state, and if not then the next state remains unchanged from the previous one. However, if we can easily generate X_I conditional both on the values of $X_j, j \neq \mathbf{I}$ and on the condition that $X \in A$, then the Gibbs sampler may be performed by doing this generation and then obtaining the next state of the Markov chain by replacing the old value of X_I by the value generated. This is illustrated by our next example.

Example 4.34 Let X_i, $i = 1, \ldots, n$ be independent random variables with X_i having an exponential distribution with rate λ_i, $i = 1, \ldots, n$. Let $S = \sum_{i=1}^{n} X_i$ and suppose that we want to generate the random vector $X = (X_1, \ldots, X_n)$ conditional on the event that $S > c$ for some large positive constant c. That is, we want to generate the value of a random vector whose density function is given by

$$f(x_1, \ldots, x_n) = \frac{1}{P\{S > c\}} \prod_{i=1}^{n} \lambda_i e^{-\lambda_i x_i} \qquad \text{if } \sum_{i=1}^{n} x_i > c$$

This is easily accomplished by starting with an initial vector $\mathbf{x} = (x_1, \ldots, x_n)$ satisfying $x_i > 0$, $i = 1, \ldots, n$ and $\sum_{i=1}^{n} x_i > c$. Then generate a variable $\mathbf{I}$

that is equally likely to be any of $1, \ldots, n$. Now, we want to generate an exponential random variable X with rate λ_I, conditioned on the event that $X + \sum_{j \neq I} x_j > c$. That is, we want to generate the value of X conditional on the event that it exceeds $c - \sum_{j \neq I} x_j$. Hence, using the fact that an exponential conditioned to be greater than a positive constant is distributed as the constant plus the exponential, we see that we should generate an exponential random variable Y with rate λ_I, and set

$$X = Y + \left(c - \sum_{j \neq I} x_j\right)^+$$

where b^+ is equal to b when $b > 0$ and is 0 otherwise. The value of x_I should then be reset to equal X and a new iteration of the algorithm begun. ◆

Remark As can be seen by Examples **4.33** and **4.34**, although the theory for the Gibb's sampler was presented under the assumption that the distribution to be generated was discrete, it also holds when this distribution is continuous.

4.10. Markov Decision Processes

Consider a process that is observed at discrete time points to be in any one of M possible states, which we number by $1, 2, \ldots, M$. After observing the state of the process, an action must be chosen, and we let A, assumed finite, denote the set of all possible actions.

If the process is in state i at time n and action a is chosen, then the next state of the system is determined according to the transition probabilities $P_{ij}(a)$. If we let X_n denote the state of the process at time n and a_n the action chosen at time n, then the above is equivalent to stating that

$$P\{X_{n+1} = j \mid X_0, a_0, X_1, a_1, \ldots, X_n = i, a_n = a\} = P_{ij}(a)$$

Thus, the transition probabilities are functions only of the present state and the subsequent action.

By a policy, we mean a rule for choosing actions. We shall restrict ourselves to policies which are of the form that the action they prescribe at any time depends only on the state of the process at that time (and not on any information concerning prior states and actions). However, we shall allow the policy to be "randomized" in that its instructions may be to choose actions according to a probability distribution. In other words, a policy $\boldsymbol{\beta}$ is a set of numbers $\boldsymbol{\beta} = \{\beta_i(a), a \in A, i = 1, \ldots, M\}$ with the interpretation that if the process is in state i, then action a is to be chosen with probability $\beta_i(a)$. Of course, we need have that

$$0 \leq \beta_i(a) \leq 1, \qquad \text{for all i,a}$$
$$\sum_a \beta_i(a) = 1, \qquad \text{for all i}$$

Under any given policy β, the sequence of states $\{X_n, n = 0, 1, \ldots\}$ constitutes a Markov chain with transition probabilities $P_{ij}(\beta)$ given by

$$\begin{aligned} P_{ij}(\beta) &= P_\beta\{X_{n+1} = j \mid X_n = i\}^* \\ &= \sum_a P_{ij}(a)\beta_i(a) \end{aligned}$$

where the last equality follows by conditioning on the action chosen when in state i. Let us suppose that for every choice of a policy β, the resultant Markov chain $\{X_n, n = 0, 1, \ldots\}$ is ergodic.

For any policy β, let π_{ia} denote the limiting (or steady-state) probability that the process will be in state i and action a will be chosen if policy β is employed. That is,

$$\pi_{ia} = \lim_{n \to \infty} P_\beta\{X_n = \text{i, a}, = \text{a}]$$

The vector $\pi = (\pi_{ia})$ must satisfy

(i) $\pi_{ia} \geq 0$ for all i, a
(ii) $\sum_i \sum_a \pi_{ia} = 1$
(iii) $\sum_a \pi_{ja} = \sum_i \sum_a \pi_{ia} P_{ij}(a)$ for all j **(4.33)**

Equations (i) and (ii) are obvious, and Equation (iii) which is an analogue of Equation (4.7) follows as the left-hand side equals the steady-state probability of being in state j and the right-hand side is the same probability computed by conditioning on the state and action chosen one stage earlier.

Thus for any policy β, there is a vector $\pi = (\pi_{ia})$ which satisfies (i)–(iii) and with the interpretation that π_{ia} is equal to the steady-state probability of being in state i and choosing action a when policy β is employed. Moreover, it turns out that the reverse is also true. Namely, for any vector $\pi = (\pi_{ia})$ which satisfies (i)–(iii), there exists a policy β such that if β is used, then the steady-state probability of being in i and choosing action a equals π_{ia}. To verify this last statement, suppose that $\pi = (\pi_{ia})$ is a vector which satisfies (i)–(iii). Then, let the policy $\beta = (\beta_i(a))$ be

$$\begin{aligned} \beta_i(a) &= P\{\beta \text{ chooses a} \mid \text{state is } i\} \\ &= \frac{\pi_{ia}}{\sum_a \pi_{ia}} \end{aligned}$$

* We use the notation P_β to signify that the probability is conditional on the fact that policy β is used.

Now let P_{ia} denote the limiting probability of being in i and choosing a when policy $\boldsymbol{\beta}$ is employed. We need to show that $P_{ia} = \pi_{ia}$. To do so, first note that $\{P_{ia}, i = 1, \ldots, M, a \in A\}$ are the limiting probabilities of the two-dimensional Markov chain $\{(X_n, a_n), n \geq 0\}$. Hence, by the fundamental Theorem 4.1, they are the unique solution of

(i') $P_{ia} \geq 0$
(ii') $\sum_i \sum_a P_{ia} = 1$
(iii') $P_{ja} = \sum_i \sum_{a'} P_{ia'} P_{ij}(a') \beta_j(a)$

where (iii') follows since

$$P\{X_{n+1} = j, a_{n+1} = a \mid X_n = i, a_n = a'\} = P_{ij}(a')\beta_j(a)$$

Since

$$\beta_j(a) = \frac{\pi_{ja}}{\sum_a \pi_{ja}}$$

we see that (P_{ia}) is the unique solution of

$$P_{ia} \geq 0,$$

$$\sum_i \sum_a P_{ia} = 1,$$

$$P_{ja} = \sum_i \sum_{a'} P_{ia'} P_{ij}(a') \frac{\pi_{ja}}{\sum_a \pi_{ja}}$$

Hence, to show that $P_{ia} = \pi_{ia}$, we need show that

$$\pi_{ia} \geq 0,$$

$$\sum_i \sum_a \pi_{ia} = 1,$$

$$\pi_{ja} = \sum_i \sum_{a'} \pi_{ia'} P_{ij}(a') \frac{\pi_{ja}}{\sum_a \pi_{ja}}$$

The top two equations follow from (i) and (ii) of Equation (4.33), and the third which is equivalent to

$$\sum_a \pi_{ja} = \sum_i \sum_{a'} \pi_{ia'} P_{ij}(a')$$

follows from condition (iii) of Equation (4.33).

Thus we have shown that a vector $\pi = (\pi_{ia})$ will satisfy (i), (ii), and (iii) of Equation (4.33) if and only if there exists a policy $\boldsymbol{\beta}$ such that π_{ia} is equal to the steady-state probability of being in state i and choosing action a when $\boldsymbol{\beta}$ is used. In fact, the policy $\boldsymbol{\beta}$ is defined by $\boldsymbol{\beta}_i(a) = \pi_{ia}/\sum_a \pi_{ia}$.

The preceding is quite important in the determination of "optimal" policies. For instance, suppose that a reward $R(i, a)$ is earned whenever action a is chosen in state i. Since $R(X_i, a_i)$ would then represent the reward earned at time i, the expected average reward per unit time under policy β can be expressed as

$$\text{expected average reward under } \boldsymbol{\beta} = \lim_{n\to\infty} E_\beta\left[\frac{\sum_{i=1}^{n} R(X_i, a_i)}{n}\right]$$

Now, if π_{ia} denotes the steady-state probability of being in state i and choosing action a, it follows that the limiting expected reward at time n equals

$$\lim_{n\to\infty} E[R(X_n, a_n)] = \sum_i \sum_a \pi_{ia} R(i, a)$$

which implies (see Exercise 60) that

$$\text{expected average reward under } \boldsymbol{\beta} = \sum_i \sum_a \pi_{ia} R(i, a)$$

Hence, the problem of determining the policy that maximizes the expected average reward is

$$\begin{aligned}
&\underset{\pi = (\pi_{ia})}{\text{maximize}} \sum_i \sum_a \pi_{ia} R(i, a) \\
&\text{subject to } \pi_{ia} \geq 0, \qquad \text{for all } i, a, \\
&\qquad \sum_i \sum_a \pi_{ia} = 1, \\
&\qquad \sum_a \pi_{ja} = \sum_i \sum_a \pi_{ia} P_{ij}(a), \qquad \text{for all } j
\end{aligned} \tag{4.34}$$

However, the above maximization problem is a special case of what is known as a linear program* and can thus be solved by a standard linear programming algorithm known as the simplex algorithm. If $\boldsymbol{\pi}^* = (\pi_{ia}^*)$ maximizes the preceding, then the optimal policy will be given by $\boldsymbol{\beta}^*$ where

$$\beta_i^*(a) = \frac{\pi_{ia}^*}{\sum_a \pi_{ia}^*}$$

Remarks (i) It can be shown that there is a $\boldsymbol{\pi}^*$ maximizing Equation (4.34) that has the property that for each i, π_{ia}^* is zero for all but one value of a, which implies that the optimal policy is nonrandomized. That is, the action it prescribes when in state i is a deterministic function of i.

* It is called a linear program since the objective function $\sum_i \sum_a R(i, a)\pi_{ia}$ and the constraints are all linear functions of the π_{ia}.

(ii) The linear programming formulation also often works when there are restrictions placed on the class of allowable policies. For instance, suppose there is a restriction on the fraction of time the process spends in some state, say, state 1. Specifically, suppose that we are only allowed to consider policies having the property that their use results in the process being in state 1 less that 100α percent of time. To determine the optimal policy subject to this requirement, we add to the linear programming problem the additional constraint

$$\sum_{a} \pi_{1a} \leq \alpha$$

since $\sum_a \pi_{1a}$ represents the proportion of time that the process is in state 1.

Exercises

***1.** Three white and three black balls are distributed in two urns in such a way that each contains three balls. We say that the system is in state i, $i = 0, 1, 2, 3,$ if the first urn contains i white balls. At each step, we draw one ball from each urn and place the ball drawn from the first urn into the second, and conversely with the ball from the second urn. Let X_n denote the state of the system after the nth step. Explain why $\{X_n, n = 0, 1, 2, \ldots\}$ is a Markov chain and calculate its transition probability matrix.

2. Suppose that whether or not it rains today depends on previous weather conditions through the last three days. Show how this system may be analyzed by using a Markov chain. How many states are needed?

3. In Exercise 2, suppose that if it has rained for the past three days, then it will rain today with probability 0.8; if it did not rain for any of the past three days, then it will rain today with probability 0.2; and in any other case the weather today will, with probability 0.6, be the same as the weather yesterday. Determine P for this Markov chain.

***4.** Consider a process $\{X_n, n = 0, 1, \ldots)$ which takes on the values 0, 1, or 2. Suppose

$$P\{X_{n+1} = j \mid X_n = i, X_{n-1} = i_{n-1}, \ldots, X_0 = i_0\} = \begin{cases} P_{ij}^{\mathrm{I}}, & \text{when } n \text{ is even} \\ P_{ij}^{\mathrm{II}}, & \text{when } n \text{ is odd} \end{cases}$$

where $\sum_{j=0}^{2} P_{ij}^{\mathrm{I}} = \sum_{j=0}^{2} P_{ij}^{\mathrm{II}} = 1, i = 0, 1, 2$. Is $\{X_n, n \geq 0\}$ a Markov chain? If not, then show how, by enlarging the state space, we may transform it into a Markov chain.

5. Let the transition probability matrix of a two-state Markov chain be given, as in Example 4.2, by

$$\mathbf{P} = \begin{Vmatrix} p & 1-p \\ 1-p & p \end{Vmatrix}$$

Show by mathematical induction that

$$\mathbf{P}^{(n)} = \begin{Vmatrix} \frac{1}{2} + \frac{1}{2}(2p-1)^n & \frac{1}{2} - \frac{1}{2}(2p-1)^n \\ \frac{1}{2} - \frac{1}{2}(2p-1)^n & \frac{1}{2} + \frac{1}{2}(2p-1)^n \end{Vmatrix}$$

6. In Example 4.4 suppose that it has rained neither yesterday nor the day before yesterday. What is the probability that it will rain tomorrow?

7. Suppose that coin 1 has probability 0.7 of coming up heads, and coin 2 has probability 0.6 of coming up heads. If the coin flipped today comes up heads, then we select coin 1 to flip tomorrow, and if it comes up tails, then we select coin 2 to flip tomorrow. If the coin initially flipped is equally likely to be coin 1 or coin 2, then what is the probability that the coin flipped on the third day after the initial flip is coin 1?

8. Specify the classes of the following Markov chains, and determine whether they are transient or recurrent:

$$\mathbf{P}_1 = \begin{Vmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{Vmatrix} \qquad \mathbf{P}_2 = \begin{Vmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \end{Vmatrix}$$

$$\mathbf{P}_3 = \begin{Vmatrix} \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{Vmatrix} \qquad \mathbf{P}_4 = \begin{Vmatrix} \frac{1}{4} & \frac{3}{4} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{3} & \frac{2}{3} & 0 \\ 1 & 0 & 0 & 0 & 0 \end{Vmatrix}$$

9. Prove that if the number of states in a Markov chain is M, and if state j can be reached from state *i,* then it can be reached in M steps or less.

'10. Show that if state i is recurrent and state i does not communicate with state j, then $P_{ij} = 0$. This implies that once a process enters a recurrent class of states it can never leave that class. For this reason, a recurrent class is often referred to as a closed class.

11. For the random walk of Example 4.13 use the strong law of large numbers to give another proof that the Markov chain is transient when $p \neq \frac{1}{2}$.

Hint: Note that the state at time n can be written as $\sum_{i=1}^{n} Y_i$ where the Y_i's are independent and $P\{Y_i = 1) = p = 1 - P\{Y_i = -1)$. Argue that if $p > \frac{1}{2}$, then, by the strong law of large numbers, $\sum_1^n Y_i \to \infty$ as $n \to \infty$ and hence the initial state 0 can be visited only finitely often, and hence must be transient. A similar argument holds when $p < \frac{1}{2}$.

12. Coin 1 comes up heads with probability 0.6 and coin 2 with probability 0.5. A coin is continually flipped until it comes up tails, at which time that coin is put aside and we start flipping the other one.

(a) What proportion of flips use coin 1?
(b) If we start the process with coin 1 what is the probability that coin 2 is used on the fifth flip?

13. For Example 4.4, calculate the proportion of days that it rains.

14. A transition probability matrix P is said to be doubly stochastic if the sum over each column equals one; that is,

$$\sum_i P_{ij} = 1, \qquad \text{for all j}$$

If such a chain is irreducible and aperiodic and consists of M + 1 states 0, 1, ..., M, show that the limiting probabilities are given by

$$\pi_j = \frac{1}{M+1}, \qquad j = 0, 1, \ldots, M$$

***15.** A particle moves on a circle through points which have been marked 0, 1, 2, 3, 4 (in a clockwise order). At each step it has a probability p of moving to the right (clockwise) and 1 − p to the left (counterclockwise). Let X_n denote its location on the circle after the nth step. The process $(X_n, n \geq 0\}$ is a Markov chain.

(a) Find the transition probability matrix.
(b) Calculate the limiting probabilities.

16. Let Y_n be the sum of n independent rolls of a fair die. Find

$$\lim_{n \to \infty} P\{Y_n \text{ is a multiple of } 13)$$

Hint: Define an appropriate Markov chain and apply the results of Exercise 14.

17. Each morning an individual leaves his house and goes for a run. He is equally likely to leave either from his front or back door. Upon leaving the house, he chooses a pair of running shoes (or goes running barefoot if there are no shoes at the door from which he departed). On his return he is equally likely to enter, and leave his running shoes, either by the front or back door. If he owns a total of k pairs of running shoes, what proportion of the time does he run barefooted?

18. Consider the following approach to shuffling a deck of n cards. Starting with any initial ordering of the cards, one of the numbers $1, 2, \ldots, n$ is randomly chosen in such a manner that each one is equally likely to be selected. If number i is chosen, then we take the card that is in position i and put it on top of the deck—that is, we put that card in position 1. We then repeatedly perform the same operation. Show that, in the limit, the deck is perfectly shuffled in the sense that the resultant ordering is equally likely to be any of the n! possible orderings.

***19.** Determine the limiting probabilities π_j for the model presented in Exercise 1. Give an intuitive explanation of your answer.

20. For a series of dependent trials the probability of success on any trial is $(k+1)/(k+2)$ where k is equal to the number of successes on the previous two trials. Compute $\lim_{n\to\infty} P\{\text{success on the nth trial}\}$.

21. An organization has N employees where N is a large number. Each employee has one of three possible job classifications and changes classifications (independently) according to a Markov chain with transition probabilities

$$\begin{bmatrix} 0.7 & 0.2 & 0.1 \\ 0.2 & 0.6 & 0.2 \\ 0.1 & 0.4 & 0.5 \end{bmatrix}$$

What percentage of employees are in each classification?

22. Three out of every four trucks on the road are followed by a car, while only one out of every five cars is followed by a truck. What fraction of vehicles on the road are trucks?

23. A certain town never has two sunny days in a row. Each day is classified as being either sunny, cloudy (but dry), or rainy. If it is sunny one day, then it is equally likely to be either cloudy or rainy the next day. If it is rainy or cloudy one day, then there is one chance in two that it will be the same the next day, and if it changes then it is equally likely to be either of the other two possibilities. In the long run, what proportion of days are sunny? What proportion are cloudy?

***24.** Each of two switches is either on or off during a day. On day n, each switch will independently be on with probability

$$[1 + \text{number of on switches during day } n - 1]/4$$

For instance, if both switches are on during day $n - 1$, then each will independently be on during day n with probability $3/4$. What fraction of days are both switches on? What fraction are both off?

25. A professor continually gives exams to her students. She can give three possible types of exams, and her class is graded as either having done well or badly. Let p_i denote the probability that the class does well on a type i exam, and suppose thatp, $= 0.3$, $p_2 = 0.6$, and $p_3 = 0.9$. If the class does well on an exam, then the next exam is equally likely to be any of the three types. If the class does badly, then the next exam is always type 1. What proportion of exams are type i, $i = 1, 2, 3$?

26. A flea moves around the vertices of a triangle in the following manner: Whenever it is at vertex i it moves to its clockwise neighbor vertex with probability p_i and to the counterclockwise neighbor with probability $q_i = 1 - p_i$, $i = 1, 2, 3$.

(a) Find the proportion of time that the flea is at each of the vertices.
(b) How often does the flea make a counterclockwise move which is then followed by 5 consecutive clockwise moves?

27. Consider a Markov chain with states 0, 1, 2, 3, 4. Suppose $P_{0,4} = 1$; and suppose that when the chain is in state i, i > 0, the next state is equally likely to be any of the states 0, 1, ..., i − 1. Find the limiting probabilities of this Markov chain.

***28.** Let π_i denote the long-run proportion of time a given Markov chain is in state i.

(a) Explain why π_i is also the proportion of transitions that are into state i as well as being the proportion of transitions that are from state i.
(b) $\pi_i P_{ij}$ represents the proportion of transitions that satisfy what property?
(c) $\sum_i \pi_i P_{ij}$ represent the proportion of transitions that satisfy what property?
(d) Using the preceding explain why

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

29. Let A be a set of states, and let A^C be the remaining states.

(a) What is the interpretation of

$$\sum_{i \in A} \sum_{j \in A^c} \pi_i P_{ij}?$$

(b) What is the interpretation of

$$\sum_{i \in A^c} \sum_{j \in A} \pi_i P_{ij}?$$

(c) Explain the identity

$$\sum_{i \in A} \sum_{j \in A^c} \pi_i P_{ij} = \sum_{i \in A^c} \sum_{j \in A} \pi_i P_{ij}$$

30. Each day, one of n possible elements is requested, the ith one with probability P_i, i ≥ 1, $\sum_1^n P_i = 1$. These elements are at all times arranged in an ordered list which is revised as follows: The element selected is moved to the front of the list with the relative positions of all the other elements remaining unchanged. Define the state at any time to be the list ordering at that time and note that there are n! possible states.

(a) Argue that the preceding is a Markov chain.
(b) For any state i,, ..., i_n (which is a permutation of 1, 2, ..., n), let $\pi(i_1, \ldots, i_n)$ denote the limiting probability. In order for the state to be i,, ..., i_n, it is necessary for the last request to be for i,, the last non-i, request for i_2, the last non-i, or i_2 request for i,, and so on. Hence, it appears intuitive that

$$\pi(i_1, \ldots, i_n) = P_{i_1} \frac{P_{i_2}}{1 - P_{i_1}} \frac{P_{i_3}}{1 - P_{i_1} - P_{i_2}} \cdots \frac{P_{i_{n-1}}}{1 - P_{i_1} - \cdots - P_{i_{n-2}}}$$

Verify when $n = 3$ that the above are indeed the limiting probabilities.

31. Suppose that a population consists of a fixed number, say, rn, of genes in any generation. Each gene is one of two possible genetic types. If any generation has exactly i (of its rn) genes being type 1, then the next generation will have j type 1 (and m − j type 2) genes with probability

$$\binom{m}{j}\left(\frac{i}{m}\right)^j \left(\frac{m-i}{m}\right)^{m-j}, \qquad j = 0, 1, \ldots, m$$

Let X_n denote the number of type 1 genes in the nth generation, and assume that $X_0 = i$.

(a) Find $E[X_n]$.
(b) What is the probability that eventually all the genes will be type 1?

32. Consider an irreducible finite Markov chain with states $0, 1, \ldots, N$.

(a) Starting in state i, what is the probability the process will ever visit state j ? Explain!
(b) Let $x_i = P\{\text{visit state N before state } 0 | \text{start in } i)$. Compute a set of linear equations which the x_i satisfy, $i = 0, 1, \ldots, N$.
(c) If $\sum_j jp_{ij} = i$ for $i = 1, \ldots, N - 1$, show that $x_i = i/N$ is a solution to the equations in part (b).

33. An individual possesses r umbrellas which he employs in going from his home to office, and vice versa. If he is at home (the office) at the beginning (end) of a day and it is raining, then he will take an umbrella with him to the office (home), provided there is one to be taken. If it is not raining, then he never takes an umbrella. Assume that, independent of the past, it rains at the beginning (end) of a day with probability p.

(i) Define a Markov chain with $r + 1$ states which will help us to determine the proportion of time that our man gets wet. (Note: He gets wet if it is raining, and all umbrellas are at his other location.)
(ii) Show that the limiting probabilities are given by

$$\pi_i = \begin{cases} \dfrac{q}{r + q}, & \text{if } i = 0 \\ \dfrac{1}{r + q}, & \text{if } i = 1, \ldots, r \end{cases} \qquad \text{where } q = 1 - p$$

(iii) What fraction of time does our man get wet?
(iv) When $r = 3$, what value of p maximizes the fraction of time he gets wet?

***34.** Let $\{X_n, n \geq 0)$ denote an **ergodic** Markov chain with limiting probabilities n. Define the process $\{Y_n, n \geq 1\}$ by $Y_n = (X_{n-1}, X_n)$. That is, Y_n keeps track of the last two states of the original chain. Is $\{Y_n, n \geq 1\}$ a Markov chain? If so, determine its transition probabilities and find

$$\lim_{n \to \infty} P\{Y_n = (i, j))$$

35. Verify the transition probability matrix given in Example 4.18.

36. Let $P^{(1)}$ and $P^{(2)}$ denote transition probability matrices for **ergodic** Markov chains having the same state space. Let π^1 and π^2 denote the stationary (limiting) probability vectors for the two chains. Consider a process defined as follows:

(i) $X_0 = 1$. A coin is then flipped and if it comes up heads, then the remaining states $X_1, \ldots$ are obtained from the transition probability matrix $P^{(1)}$ and if tails from the matrix $P^{(2)}$. Is $\{X_n, n \geq 0\}$ a Markov chain? If $p = P\{\text{coin comes up heads}\}$, what is $\lim_{n\to\infty} P(X_n = i)$?
(ii) $X_0 = 1$. At each stage the coin is flipped and if it comes up heads, then the next state is chosen according to $P^{(1)}$ and if tails comes up, then it is chosen according to $P^{(2)}$. In this case do the successive states constitute a Markov chain? If so, determine the transition probabilities. Show by a counterexample that the limiting probabilities are not the same as in part (i).

37. A fair coin is continually flipped. Compute the expected number of flips until the following patterns appear:

(a) HHTTHT
*(b) HHTTHH
(c) HHTHHT

38. Consider the Ehrenfest urn model in which M molecules are distributed among two urns, and at each time point one of the molecules is chosen at random and is then removed from its urn and placed in the other one. Let X_n denote the number of molecules in urn 1 after the nth switch and let $\mu_n = E[X_n]$. Show that

(i) $\mu_{n+1} = 1 + (1 - 2/M)\mu_n$
(ii) Use (i) to prove that

$$\mu_n = \frac{M}{2} + \left(\frac{M-2}{M}\right)^n \left(E[X_0] - \frac{M}{2}\right)$$

39. Consider a population of individuals each of whom possesses two genes which can be either type A or type a. Suppose that in outward appearance type A is dominant and type a is recessive. (That is, an individual will only have the outward characteristics of the recessive gene if its pair is aa.) Suppose that the population has stabilized, and the percentages of individuals having respective gene pairs AA, aa, and Aa are p, q, and r. Call an individual dominant or recessive depending on the outward characteristics it exhibits. Let S_{11} denote the probability that an offspring of two dominant parents will be recessive; and let S_{10} denote the probability that the offspring of one dominant and one recessive parent will be recessive. Compute S_{11} and S_{10} to show that $S_{11} = S_{10}^2$. (The quantities S_{10} and S_{11} are known in the genetics literature as Snyder's ratios.)

40. Suppose that on each play of the game a gambler either wins 1 with probability p or loses 1 with probability 1 − p. The gambler continues betting until she or he is either winning n or losing m. What is the probability that the gambler quits a winner?

41. A particle moves among n + 1 vertices that are situated on a circle in the following manner: At each step it moves one step either in the clockwise direction with probability p or the counterclockwise direction with probability q = 1 − p. Starting at a specified state, call it state **0**, let T be the time of the first return to state **0**. Find the probability that all states have been visited by time T.

Hint: Condition on the initial transition and then use results from the gambler's ruin problem.

42. In the gambler's ruin problem of Section 4.5.1, suppose the gambler's fortune is presently i, and suppose that we know that the gambler's fortune will eventually reach N (before it goes to **0**). Given this information, show that the probability he wins the next gamble is

$$\frac{p[1-(q/p)^{i+1}]}{1-(q/p)^i}, \qquad \text{if } p \neq \tfrac{1}{2}$$

$$\frac{i+1}{2i}, \qquad \text{if } p = \tfrac{1}{2}$$

Hint: The probability we want is

$$P\{X_{n+1} = i+1 \mid X_n = i, \lim_{m\to\infty} X_m = N\}$$

$$= \frac{P\{X_{n+1} = i+1, \lim_m X_m = N \mid X_n = i\}}{P\{\lim_m X_m = N \mid X_n = i\}}$$

43. For the gambler's ruin model of Section 4.5.1, let M_i denote the mean number of games that must be played until the gambler either goes broke or reaches a fortune of N, given that he starts with i, i = 0, 1, ..., N. Show that M_i satisfies

$$M_0 = M_N = 0; \qquad M_i = 1 + pM_{i+1} + qM_{i-1}, \qquad i = 1, \ldots, N-1$$

44. Solve the equations given in Exercise **43** to obtain

$$M_i = i(N-i), \qquad \text{if } p = \tfrac{1}{2}$$

$$= \frac{i}{q-p} - \frac{N}{q-p}\frac{1-(q/p)^i}{1-(q/p)^N}, \qquad \text{if } p \neq \tfrac{1}{2}$$

'45. In Exercise 15,

(a) what is the expected number of steps the particle takes to return to the starting position?
(b) what is the probability that all other positions are visited before the particle returns to its starting state?

46. For the Markov chain with states $1, 2, 3, 4$ whose transition probability matrix P is as specified below find f_{i3} and s_{i3} for $i = 1, 2, 3$.

$$\mathbf{P} = \begin{bmatrix} 0.4 & 0.2 & 0.1 & 0.3 \\ 0.1 & 0.5 & 0.2 & 0.2 \\ 0.3 & 0.4 & 0.2 & 0.1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

47. Consider a branching process having $\mu < 1$. Show that if $X_0 = 1$, then the expected number of individuals that ever exist in this population is given by $1/(1 - \mu)$. What if $X_0 = n$?

48. In a branching process having $X_0 = 1$ and $\mu > 1$, prove that π_0 is the ***smallest*** positive number satisfying Equation (4.15).

Hint: Let π be any solution of $\pi = \sum_{j=0}^{\infty} \pi^j P_j$. Show by mathematical induction that $\pi \geq P\{X_n = 0\}$ for all n, and let $n \to \infty$. In using the induction argue that

$$P\{X_n = 0) = \sum_{j=0}^{\infty} (P\{X_{n-1} = 0\})^j P_j$$

49. For a branching process, calculate π_0 when

(a) $P_0 = \frac{1}{4}$, $P_2 = \frac{3}{4}$
(b) $P_0 = \frac{1}{4}$, $P_1 = \frac{1}{2}$, $P_2 = \frac{1}{4}$
(c) $P_0 = \frac{1}{6}$, $P_1 = \frac{1}{2}$, $P_3 =$ f-

50. At all times, an urn contains N balls—some white balls and some black balls. At each stage, a coin having probability p, $0 < p < 1$, of landing heads is flipped. If heads appears, then a ball is chosen at random from the urn and is replaced by a white ball; if tails appears, then a ball is chosen from the urn and is replaced by a black ball. Let X_n denote the number of white balls in the urn after the nth stage.

(a) Is $\{X_n, n \geq 0\}$ a Markov chain? If so, explain why.
(b) What are its classes? What are their periods? Are they transient or recurrent?
(c) Compute the transition probabilities P_{ij}.
(d) Let $N = 2$. Find the proportion of time in each state.
(e) Based on your answer in part (d) and your intuition, guess the answer for the limiting probability in the general case.
(f) Prove your guess in part (e) either by showing that Equation (4.7) is satisfied or by using the results of Example 4.28.
(g) If $p = 1$, what is the expected time until there are only white balls in the urn if initially there are i white and $N - i$ black?

***51.** (a) Show that the limiting probabilities of the reversed Markov chain are the same as for the forward chain by showing that they satisfy the equations

$$\pi_j = \sum_i \pi_i Q_{ij}$$

(b) Give an intuitive explanation for the result of part (a).

52. M balls are initially distributed among m urns. At each stage one of the balls is selected at random, taken from whichever urn it is in, and then placed, at random, in one of the other $M - 1$ urns. Consider the Markov chain whose state at any time is the vector $(n_1, \ldots, n_m)$ where n_i denotes the number of balls in urn i. Guess at the limiting probabilities for this Markov chain and then verify your guess and show at the same time that the Markov chain is time reversible.

53. It follows from Theorem 4.2 that for a time reversible Markov chain

$$P_{ij}P_{jk}P_{ki} = P_{ik}P_{kj}P_{ji}, \qquad \text{for all } i, j, k$$

It turns out that if the state space is finite and $P_{ij} > 0$ for all i, j, then the preceding is also a sufficient condition for time reversibility. (That is, in this case, we need only check Equation (4.26) for paths from i to i that have only two intermediate states.) Prove this.

Hint: Fix i and show that the equations

$$\pi_j P_{jk} = \pi_k P_{kj}$$

are satisfied by $\pi_j = cP_{ij}/P_{ji}$, where c is chosen so that $\sum_j \pi_j = 1$.

54. For a time reversible Markov chain, argue that the rate at which transitions from i to j to k occur must equal the rate at which transitions from k to j to i occur.

55. Show that the Markov chain of Exercise **23** is time reversible.

56. A group of n processors are arranged in an ordered list. When a job arrives, the first processor in line attempts it; if it is unsuccessful, then the next in line tries it; if it too is unsuccessful, then the next in line tries it, and so on. When the job is successfully processed or after all processors have been unsuccessful, the job leaves the system. At this point we are allowed to reorder the processors, and a new job appears. Suppose that we use the one-closer reordering rule, which moves the processor that was successful one closer to the front of the line by interchanging its position with the one in front of it. If all processors were unsuccessful (or if the processor in the first position was successful), then the ordering remains the same. Suppose that each time processor i attempts a job then, independently of anything else, it is successful with probability p_i.

(a) Define an appropriate Markov chain to analyze this model.
(b) Show that this Markov chain is time reversible.
(c) Find the long run probabilities.

57. A Markov chain is said to be a tree process if

(i) $P_{ij} > 0$ whenever $P_{ji} > 0$.
(ii) for every pair of states i and j, $i \neq j$, there is a unique sequence of distinct states $i = i_0, i_1, \ldots, i_{n-1}, i_n = j$ such that

$$P_{i_k, i_{k+1}} > 0, \qquad k = 0, 1, \ldots, n-1$$

In other words, a Markov chain is a tree process if for every pair of distinct states i and j there is a unique way for the process to go from i to j without reentering a state (and this path is the reverse of the unique path from j to i). Argue that an **ergodic** tree process is time reversible.

58. On a chessboard compute the expected number of plays it takes a knight, starting in one of the four corners of the chessboard, to return to its initial position if we assume that at each play it is equally likely to choose any of its legal moves. (No other pieces are on the board.)

Hint: Make use of Example **4.29.**

59. In a Markov decision problem, another criterion often used, different than the expected average return per unit time, is that of the expected discounted return. In this criterion we choose a number a, $0 < a < 1$, and try to choose a policy so as to maximize $E[\sum_{i=0}^{\infty} \alpha^i R(X_i, a_i)]$. (That is, rewards at time n are discounted at rate a^n.) Suppose that the initial state is chosen according to the probabilities b_i. That is,

$$P\{X_0 = i\} = b_i, \qquad i = 1, \ldots, n$$

For a given policy β let y_{ja} denote the expected discounted time that the process is in state j and action a is chosen. That is,

$$y_{ja} = E_\beta\left[\sum_{n=0}^{\infty} \alpha^n I_{\{X_n = j, a_n = a\}}\right]$$

where for any event A the indicator variable I_A is defined by

$$I_A = \begin{cases} 1, & \text{if A occurs} \\ 0, & \text{otherwise} \end{cases}$$

(a) Show that

$$\sum_a y_{ja} = E\left[\sum_{n=0}^{\infty} \alpha^n I_{\{X_n = j\}}\right]$$

or, in other words, $\sum_a y_{ja}$ is the expected discounted time in state j under β.

(b) Show that

$$\sum_j \sum_a y_{ja} = \frac{1}{1-\alpha},$$

$$\sum_a Y_{ja} = b_j + \alpha \sum_i \sum_a y_{ia} P_{ij}(a)$$

Hint: For the second equation, use the identity

$$I_{\{X_{n+1} = j\}} = \sum_i \sum_a I_{\{X_n = i, a_n = a\}} I_{\{X_{n+1} = j\}}$$

Take expectations of the preceding to obtain

$$E[I_{\{X_{n+1} = j\}}] = \sum_i \sum_a E[I_{\{X_n = i, a_n = a\}}] P_{ij}(a).$$

(c) Let $\{y_{ja}\}$ be a set of numbers satisfying

$$\sum_j \sum_a y_{ja} = \frac{1}{1-\alpha}$$

$$\sum_a Y_{ja} = b_j + \alpha \sum_i \sum_a y_{ia} P_{ij}(a) \qquad \textbf{(4.35)}$$

Argue that y_{ja} can be interpreted as the expected discounted time that the process is in state j and action a is chosen when the initial state is chosen according to the probabilities b_j and the policy β, given by

$$\beta_i(a) = \frac{Y_{ia}}{C_a y_{ia}}$$

is employed.

Hint: Derive a set of equations for the expected discounted times when policy β is used and show that they are equivalent to Equation (4.35).

(d) Argue that an optimal policy with respect to the expected discounted return criterion can be obtained by first solving the linear program

$$\text{maximize} \quad \sum_j \sum_a y_{ja} R(j, a),$$

$$\text{such that} \quad \sum_j \sum_a y_{ja} = \frac{1}{1-\alpha},$$

$$\sum_a y_{ja} = b_j + \alpha \sum_i \sum_a y_{ia} P_{ij}(a),$$

$$y_{ja} \geq 0, \qquad \text{all } j, a;$$

and then defining the policy β^* by

$$\beta_i^*(a) = \frac{y_{ia}^*}{\sum_a y_{ia}^*}$$

where the y_{ja}^* are the solutions of the linear program.

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