7

Discrete-Time Markov Chains

7.1 Introduction

Applied probability thrives on models. Markov chains are one of the richest sources of good models for capturing dynamical behavior with a large stochastic component [23, 24, 59, 80, 106, 107, 118]. In this chapter we give a few examples and a quick theoretical overview of discrete-time Markov chains. The highlight of our theoretical development, Proposition 7.4.1, relies on a coupling argument. Because coupling is one of the most powerful and intuitively appealing tools available to probabilists, we examine a few of its general applications as well. We also stress reversible Markov chains. Reversibility permits explicit construction of the long-run or equilibrium distribution of a chain when such a distribution exists. Chapter 8 will cover continuous-time Markov chains.

7.2 Definitions and Elementary Theory

For the sake of simplicity, we will only consider chains with a finite or countable number of states [23, 59, 80, 106, 107]. The movement of such a chain from epoch to epoch (equivalently generation to generation) is governed by its transition probability matrix $P = (p_{ij})$. This matrix is infinite dimensional when the number of states is infinite. If Z_n denotes the state of the chain at epoch n, then $p_{ij} = \Pr(Z_n = j \mid Z_{n-1} = i)$. As a consequence, every entry of P satisfies $p_{ij} \geq 0$, and every row of P satisfies

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$\sum_j p_{ij} = 1$. Implicit in the definition of p_{ij} is the fact that the future of the chain is determined by its present regardless of its past. This Markovian property is expressed formally by the equation

$$\Pr(Z_n = i_n \mid Z_{n-1} = i_{n-1}, \ldots, Z_0 = i_0) \quad = \quad \Pr(Z_n = i_n \mid Z_{n-1} = i_{n-1}).$$

The n-step transition probability $p_{ij}^{(n)} = \Pr(Z_n = j \mid Z_0 = i)$ is given by the entry in row i and column j of the matrix power P^n. This follows because the decomposition

$$p_{ij}^{(n)} \quad = \quad \sum_{i_1} \cdots \sum_{i_{n-1}} p_{ii_1} \cdots p_{i_{n-1}j}$$

over all paths $i \to i_1 \to \cdots \to i_{n-1} \to j$ of n steps corresponds to $n-1$ matrix multiplications. If the chain tends toward stochastic equilibrium, then the limit of $p_{ij}^{(n)}$ as n increases should exist independently of the starting state i. In other words, the matrix powers P^n should converge to a matrix with identical rows. Denoting the common limiting row by π, we deduce that $\pi = \pi P$ from the calculation

$$\begin{aligned}
\begin{pmatrix} \pi \\ \vdots \\ \pi \end{pmatrix} &= \lim_{n\to\infty} P^{n+1} \\
&= \Big(\lim_{n\to\infty} P^n\Big) P \\
&= \begin{pmatrix} \pi \\ \vdots \\ \pi \end{pmatrix} P.
\end{aligned}$$

Any probability distribution π on the states of the chain satisfying the condition $\pi = \pi P$ is termed an equilibrium (or stationary) distribution of the chain. The jth component

$$\pi_j \quad = \quad \sum_i \pi_i p_{ij} \tag{7.1}$$

of the equation $\pi = \pi P$ suggests a balance between the probabilistic flows into and out of state j. Indeed, if the left-hand side of equation (7.1) represents the probability of being in state j at the current epoch, then the right-hand side represents the probability of being in state j at the next epoch. At equilibrium, these two probabilities must match. For finite-state chains, equilibrium distributions always exist [59, 80]. The real issue is uniqueness.

Probabilists have attacked the uniqueness problem by defining appropriate ergodic conditions. For finite-state Markov chains, two ergodic assumptions are invoked. The first is aperiodicity; this means that the greatest common divisor of the set $\{n \geq 1 : p_{ii}^{(n)} > 0\}$ is 1 for every state i. Aperiodicity trivially holds when $p_{ii} > 0$ for all i. The second ergodic assumption is irreducibility; this means that for every pair of states (i, j), there exists a positive integer n_{ij} such that $p_{ij}^{(n_{ij})} > 0$. In other words, every state is reachable from every other state. Said yet another way, all states communicate. For a finite-state irreducible chain, Problem 4 states that the integer n_{ij} can be chosen independently of the particular pair (i, j) if and only if the chain is also aperiodic. Thus, we can merge the two ergodic assumptions into the single assumption that some power P^n has all entries positive. Under this single ergodic condition, we show in Proposition 7.4.1 that a unique equilibrium distribution π exists and that $\lim_{n\to\infty} p_{ij}^{(n)} = \pi_j$. Because all states communicate, the entries of π are necessarily positive.

Equally important is the ergodic theorem [59, 80]. This theorem permits one to run a chain and approximate theoretical means by sample means. More precisely, let $f(z)$ be some real-valued function defined on the states of an ergodic chain. Then given that Z_i is the state of the chain at epoch i and π is the equilibrium distribution, we have

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} f(Z_i) \quad = \quad \mathrm{E}_\pi[f(Z)] \quad = \quad \sum_z \pi_z f(z).$$

This result generalizes the law of large numbers for independent sampling and has important applications in Markov chain Monte Carlo methods as discussed later in this chapter. The ergodic theorem generalizes to periodic irreducible chains even though $\lim_{n\to\infty} P^n$ no longer exists. Problem 9 also indicates that uniqueness of the equilibrium distribution has nothing to do with aperiodicity.

In many Markov chain models, the equilibrium distribution satisfies the stronger condition

$$\pi_j p_{ji} \quad = \quad \pi_i p_{ij} \tag{7.2}$$

for all pairs (i, j). If this is the case, then the probability distribution π is said to satisfy detailed balance, and the Markov chain, provided it is irreducible, is said to be reversible. Summing equation (7.2) over i yields the equilibrium condition (7.1). Thus, detailed balance implies balance. Irreducibility is imposed as part of reversibility to guarantee that π is unique and has positive entries. Given the latter condition, detailed balance implies that $p_{ij} > 0$ if and only if $p_{ji} > 0$.

If $i_1, \ldots, i_m$ is any sequence of states in a reversible chain, then detailed balance also entails

$$\begin{aligned} \pi_{i_1} p_{i_1 i_2} &= \pi_{i_2} p_{i_2 i_1} \\ \pi_{i_2} p_{i_2 i_3} &= \pi_{i_3} p_{i_3 i_2} \\ &\vdots \end{aligned}$$

$$\begin{aligned}\pi_{i_{m-1}} p_{i_{m-1} i_m} &= \pi_{i_m} p_{i_m i_{m-1}} \\ \pi_{i_m} p_{i_m i_1} &= \pi_{i_1} p_{i_1 i_m}.\end{aligned}$$

Multiplying these equations together and canceling the common positive factor $\pi_{i_1} \cdots \pi_{i_m}$ from both sides of the resulting equality give Kolmogorov's circulation criterion [111]

$$p_{i_1 i_2} p_{i_2 i_3} \cdots p_{i_{m-1} i_m} p_{i_m i_1} = p_{i_1 i_m} p_{i_m i_{m-1}} \cdots p_{i_3 i_2} p_{i_2 i_1}. \tag{7.3}$$

Conversely, suppose an irreducible Markov chain satisfies Kolmogorov's criterion. One can easily demonstrate that $p_{ij} > 0$ if and only if $p_{ji} > 0$. Indeed, if $p_{ij} > 0$, then take a path of positive probability from j back to i. This creates a circuit from i to i whose first step goes from i to j. Kolmogorov's criterion shows that the reverse circuit from i to i whose last step goes from j to i also has positive probability. We can also prove that the chain is reversible by explicitly constructing the equilibrium distribution and showing that it satisfies detailed balance. The idea behind the construction is to choose some arbitrary reference state i and to pretend that π_i is given. If j is another state, let $i \to i_1 \to \cdots \to i_m \to j$ be any path leading from i to j. Then the formula

$$\pi_j = \pi_i \frac{p_{i i_1} p_{i_1 i_2} \cdots p_{i_m j}}{p_{j i_m} p_{i_m i_{m-1}} \cdots p_{i_1 i}} \tag{7.4}$$

defines π_j. A straightforward application of Kolmogorov's criterion (7.3) shows that definition (7.4) does not depend on the particular path chosen from i to j. To validate detailed balance, suppose that k is adjacent to j. Then $i \to i_1 \to \cdots \to i_m \to j \to k$ furnishes a path from i to k through j. It follows from (7.4) that

$$\pi_k = \pi_i \frac{p_{i i_1} p_{i_1 i_2} \cdots p_{i_m j} p_{jk}}{p_{j i_m} p_{i_m i_{m-1}} \cdots p_{i_1 i} p_{kj}} = \pi_j \frac{p_{jk}}{p_{kj}},$$

which is obviously equivalent to detailed balance. In general, the value of π_i is determined by the requirement that $\sum_j \pi_j = 1$. For a chain with a finite number of states, we can guarantee this condition by replacing π by $\tilde{\pi}$ with components

$$\tilde{\pi}_j = \frac{\pi_j}{\sum_k \pi_k}.$$

In practice, explicit calculation of the sum $\sum_k \pi_k$ may be nontrivial. For a chain with an infinite number of states, in contrast, it may be impossible to renormalize the π_j defined by equation (7.4) so that $\sum_j \pi_j = 1$. This situation occurs in Example 7.3.1 in the next section.

7.3 Examples

Here are a few examples of discrete-time chains classified according to the concepts just introduced. If possible, the unique equilibrium distribution is identified. For some irreducible chains, note that Kolmogorov's circulation criterion is trivial to verify. If we put an edge between two states i and j whenever $p_{ij} > 0$, then this construction induces a graph. If the graph reduces to a tree, then it can have no cycles, and Kolmogorov's circulation criterion is automatically satisfied.

Example 7.3.1 *Random Walk on a Graph*

Consider a connected graph with node set N and edge set E. The number of edges $d(v)$ incident on a given node v is called the degree of v. Owing to the connectedness assumption, $d(v) > 0$ for all $v \in N$. Now define the transition probability matrix $P = (p_{uv})$ by

$$p_{uv} = \begin{cases} \frac{1}{d(u)} & \text{for } \{u, v\} \in E \\ 0 & \text{for } \{u, v\} \notin E. \end{cases}$$

This Markov chain is irreducible because of the connectedness assumption. It is also aperiodic unless the graph is bipartite. (A graph is said to be bipartite if we can partition its node set into two disjoint subsets F and M, say females and males, such that each edge has one node in F and the other node in M.) If E has m edges, then the equilibrium distribution π of the chain has components $\pi_v = \frac{d(v)}{2m}$. It is trivial to show that this choice of π satisfies detailed balance.

One hardly needs this level of symmetry to achieve detailed balance. For instance, consider a random walk on the nonnegative integers with neighboring integers connected by an edge. For $i > 0$ let

$$p_{ij} = \begin{cases} q_i, & j = i - 1 \\ r_i, & j = i \\ p_i, & j = i + 1 \\ 0, & \text{otherwise.} \end{cases}$$

At the special state 0, set $p_{00} = r_0$ and $p_{01} = p_0$ for $p_0 + r_0 = 1$. With state 0 as a reference state, Kolmogorov's formula (7.4) becomes

$$\pi_i = \pi_0 \prod_{j=1}^{i} \frac{p_{j-1}}{q_j}.$$

This definition of π_i satisfies detailed balance because the graph of the chain is a tree. However, because the state space is infinite, we must impose the additional constraint

$$\sum_{i=0}^{\infty} \prod_{j=1}^{i} \frac{p_{j-1}}{q_j} < \infty$$

to achieve a legitimate equilibrium distribution. When this condition holds, we define

$$\pi_i = \frac{\prod_{j=1}^{i} \frac{p_{j-1}}{q_j}}{\sum_{k=0}^{\infty} \prod_{j=1}^{k} \frac{p_{j-1}}{q_j}} \tag{7.5}$$

and eliminate the unknown π_0. For instance, if all $p_j = p$ and all $q_j = q$, then $p < q$ is both necessary and sufficient for the existence of an equilibrium distribution. When $p < q$, formula (7.5) implies $\pi_i = \frac{(q-p)p^i}{q^{i+1}}$. ■

Example 7.3.2 *Wright-Fisher Model of Genetic Drift*

Consider a population of m organisms from some animal or plant species. Each member of this population carries two genes at some genetic locus, and these genes take two forms (or alleles) labeled a_1 and a_2. At each generation, the population reproduces itself by sampling $2m$ genes with replacement from the current pool of $2m$ genes. If Z_n denotes the number of a_1 alleles at generation n, then it is clear that the Z_n constitute a Markov chain with binomial transition probability matrix

$$p_{jk} = \binom{2m}{k}\Big(\frac{j}{2m}\Big)^k \Big(1 - \frac{j}{2m}\Big)^{2m-k}.$$

This chain is reducible because once one of the states 0 or $2m$ is reached, the corresponding allele is fixed in the population, and no further variation is possible. An infinity of equilibrium distributions π exist. Each one is characterized by $\pi_0 = \alpha$ and $\pi_{2m} = 1 - \alpha$ for some $\alpha \in [0, 1]$. ■

Example 7.3.3 *Ehrenfest's Model of Diffusion*

Consider a box with m gas molecules. Suppose the box is divided in half by a rigid partition with a very small hole. Molecules drift aimlessly around each half until one molecule encounters the hole and passes through. Let Z_n be the number of molecules in the left half of the box at epoch n. If epochs are timed to coincide with molecular passages, then the transition matrix of the chain is

$$p_{jk} = \begin{cases} 1 - \frac{j}{m} & \text{for } k = j + 1 \\ \frac{j}{m} & \text{for } k = j - 1 \\ 0 & \text{otherwise.} \end{cases}$$

This chain is a random walk with finite state space. It is periodic with period 2, irreducible, and reversible with equilibrium distribution

$$\pi_j = \binom{m}{j}\Big(\frac{1}{2}\Big)^m.$$

The binomial form of π_j follows from equation (7.5). ■

Example 7.3.4 *Discrete Renewal Process*

Many treatments of Markov chain theory depend on a prior development of renewal theory. Here we reverse the logical flow and consider a discrete renewal process as a Markov chain. A renewal process models repeated visits to a special state [59, 80]. After it enters the special state, the process departs and eventually returns for the first time after $j > 0$ steps with probability f_j. The return times following different visits are independent. In modeling this behavior by a Markov chain, we let Z_n denote the number of additional epochs left after epoch n until a return to the special state occurs. The renewal mechanism generates the transition matrix with entries

$$p_{ij} \quad = \quad \begin{cases} f_{j+1}, & i = 0 \\ 1, & i > 0 \text{ and } j = i-1 \\ 0, & i > 0 \text{ and } j \neq i-1. \end{cases}$$

In order for $\sum_j p_{0j} = 1$, we must have $f_0 = 0$. If $f_j = 0$ for $j > m$, then the chain has m states; otherwise, it has an infinite number of states. Because the chain always ratchets downward from $i > 0$ to $i-1$, it is both irreducible and irreversible. State 0, and therefore the whole chain, is aperiodic if and only if the set $\{j : f_j > 0\}$ has greatest common divisor 1. This number theoretic fact is covered in Appendix A.1.

One of the primary concerns in renewal theory is predicting what fraction of epochs are spent in the special state. This problem is solved by finding the equilibrium probability π_0 of state 0 in the associated Markov chain. Assuming the mean $\mu = \sum_i i f_i$ is finite, we can easily calculate the equilibrium distribution. The balance conditions defining equilibrium are

$$\pi_j \quad = \quad \pi_{j+1} + \pi_0 f_{j+1}.$$

One can demonstrate by induction that the unique solution to this system of equations is given by

$$\pi_j \quad = \quad \pi_0 \left(1 - \sum_{i=1}^{j} f_i\right) \quad = \quad \pi_0 \sum_{i=j+1}^{\infty} f_i$$

subject to

$$1 \quad = \quad \sum_{j=0}^{\infty} \pi_j \quad = \quad \pi_0 \sum_{j=0}^{\infty} \sum_{i=j+1}^{\infty} f_i \quad = \quad \pi_0 \mu.$$

Here we assume an infinite number of states and invoke Example 2.5.1. It follows that $\pi_0 = \mu^{-1}$ and $\pi_j = \mu^{-1} \sum_{i=j+1}^{\infty} f_i$.

Since the return visits to a specific state of a Markov chain constitute a renewal process, the formula $\pi_0 = \mu^{-1}$ provides an alternative way of defining the equilibrium distribution. For a symmetric random walk on the integers, the mean first passage time μ from any state back to itself is infinite. Problems 36 and 37 ask the reader to check this fact as well as the fact that the return probabilities f_n sum to 1. These observations are obviously consistent with the failure of Kolmogorov's formula (7.4) to deliver an equilibrium distribution with finite mass. Markov chains with finitely many states cannot exhibit such null recurrent behavior. ■

Example 7.3.5 *Card Shuffling and Random Permutations*

Imagine a deck of cards labeled $1, \ldots, m$. The cards taken from top to bottom provide a permutation σ of these m labels. The usual method of shuffling cards, the so-called riffle shuffle, is difficult to analyze probabilistically. A far simpler shuffle is the top-in shuffle [3, 49]. In this shuffle, one takes the top card on the deck and moves it to a random position in the deck. Of course, if the randomly chosen position is the top position, then the deck suffers no change. Repeated applications of the top-in shuffle constitute a Markov chain. This chain is aperiodic and irreducible. Aperiodicity is obvious because the deck can remain constant for an arbitrary number of shuffles. Irreducibility is slightly more subtle. Suppose we follow the card originally at the bottom of the deck. Cards inserted below it occur in completely random order. Once the original bottom card reaches the top of the deck and is moved, then the whole deck is randomly rearranged. This argument shows that all permutations are ultimately equally likely and can be reached from any starting permutation. We extend this analysis in Example 7.4.3. Finally, the chain is irreversible. For example, if a deck of seven cards is currently in the order $\sigma = (4, 7, 5, 2, 3, 1, 6)$, equating left to top and right to bottom, then inserting the top card 4 in position 3 produces $\eta = (7, 5, 4, 2, 3, 1, 6)$. Clearly, it is impossible to return from η to σ by moving the new top card 7 to another position. Under reversibility, each individual step of a Markov chain can be reversed. ■

7.4 Coupling

In this section we undertake an investigation of the convergence of an ergodic Markov chain to its equilibrium. Our method of attack exploits a powerful proof technique known as coupling. By definition, two random variables or stochastic processes are coupled if they reside on the same probability space [134, 136]. As a warm-up, we illustrate coupling arguments by two examples having little to do with Markov chains.

Example 7.4.1 *Correlated Random Variables*

Suppose X is a random variable and the functions $f(x)$ and $g(x)$ are both increasing or both decreasing. If the random variables $f(X)$ and $g(X)$ have finite second moments, then it is reasonable to conjecture that

$\text{Cov}[f(X), g(X)] \geq 0$. To prove this fact by coupling, consider a second random variable Y independent of X but sharing the same distribution. If $f(x)$ and $g(x)$ are both increasing or both decreasing, then the product $[f(X) - f(Y)][g(X) - g(Y)] \geq 0$. Hence,

$$\begin{aligned} 0 &\leq \mathrm{E}\{[f(X) - f(Y)][g(X) - g(Y)]\} \\ &= \mathrm{E}[f(X)g(X)] + \mathrm{E}[f(Y)g(Y)] - \mathrm{E}[f(X)]\,\mathrm{E}[g(Y)] - \mathrm{E}[f(Y)]\,\mathrm{E}[g(X)] \\ &= 2\,\text{Cov}[f(X), g(X)]. \end{aligned}$$

When one of the two functions is increasing and the other is decreasing, the same proof with obvious modifications shows that $\text{Cov}[f(X), g(X)] \leq 0$. ■

Example 7.4.2 *Monotonicity in Bernstein's Approximation*

In Example 3.5.1, we considered Bernstein's proof of the Weierstrass approximation theorem. When the continuous function $f(x)$ being approximated is increasing, it is plausible that the approximating polynomial

$$\mathrm{E}\left[f\left(\frac{S_n}{n}\right)\right] = \sum_{k=0}^{n} f\left(\frac{k}{n}\right)\binom{n}{k} x^k (1-x)^{n-k}.$$

is increasing as well [136]. To prove this assertion by coupling, imagine scattering n points randomly on the unit interval. If $x \leq y$ and we interpret S_n as the number of points less than or equal to x and T_n as the number of points less than or equal to y, then these two binomially distributed random variables satisfy $S_n \leq T_n$. The desired inequality

$$\mathrm{E}\left[f\left(\frac{S_n}{n}\right)\right] \leq \mathrm{E}\left[f\left(\frac{T_n}{n}\right)\right]$$

now follows directly from the assumption that f is increasing. ■

Our coupling proof of the convergence of an ergodic Markov chain depends on quantifying the distance between the distributions π_X and π_Y of two integer-valued random variables X and Y. One candidate distance is the total variation norm

$$\begin{aligned} \|\pi_X - \pi_Y\|_{\text{TV}} &= \sup_{A \subset \mathcal{Z}} |\Pr(X \in A) - \Pr(Y \in A)| \\ &= \frac{1}{2}\sum_k |\Pr(X = k) - \Pr(Y = k)|, \end{aligned} \tag{7.6}$$

where A ranges over all subsets of the integers $\mathcal{Z}$ [49]. Problem 28 asks the reader to check that these two definitions of the total variation norm are equivalent. The coupling bound

$$\|\pi_X - \pi_Y\|_{\text{TV}} = \sup_{A \subset \mathcal{Z}} |\Pr(X \in A) - \Pr(Y \in A)|$$

$$\begin{aligned}
&= \sup_{A \subset \mathcal{Z}} |\Pr(X \in A, X = Y) + \Pr(X \in A, X \neq Y) \\
&\quad - \Pr(Y \in A, X = Y) - \Pr(Y \in A, X \neq Y)| \quad (7.7) \\
&= \sup_{A \subset \mathcal{Z}} |\Pr(X \in A, X \neq Y) - \Pr(Y \in A, X \neq Y)| \\
&\leq \sup_{A \subset \mathcal{Z}} \mathrm{E}(1_{\{X \neq Y\}} |1_A(X) - 1_A(Y)|) \\
&\leq \Pr(X \neq Y)
\end{aligned}$$

has many important applications.

In our convergence proof, we actually consider two random sequences X_n and Y_n and a random stopping time T such that $X_n = Y_n$ for all $n \geq T$. The bound

$$\Pr(X_n \neq Y_n) \quad \leq \quad \Pr(T > n)$$

suggests that we study the tail probabilities $\Pr(T > n)$. By definition, a stopping time such as T relies only on the past and present and does not anticipate the future. More formally, if $\mathcal{F}_n$ is the σ-algebra of events determined by the X_i and Y_i with $i \leq n$, then $\{T \leq n\} \in \mathcal{F}_n$. In the setting of Proposition 7.4.1,

$$\Pr(T \leq n + r \mid \mathcal{F}_n) \quad \geq \quad \epsilon \tag{7.8}$$

for some $\epsilon > 0$ and $r \geq 1$ and all n. This implies the further inequality

$$\begin{aligned}
\Pr(T > n + r) &= \mathrm{E}(1_{\{T > n+r\}}) \\
&= \mathrm{E}(1_{\{T > n\}} 1_{\{T > n+r\}}) \\
&= \mathrm{E}[1_{\{T > n\}} \, \mathrm{E}(1_{\{T > n+r\}} \mid \mathcal{F}_n)] \\
&\leq \mathrm{E}[1_{\{T > n\}} (1 - \epsilon)] \\
&= (1 - \epsilon) \Pr(T > n),
\end{aligned}$$

which can be iterated to produce

$$\Pr(T > kr) \quad \leq \quad (1 - \epsilon)^k. \tag{7.9}$$

In the last step of the iteration, we must take $\mathcal{F}_0$ to be the trivial σ-algebra consisting of the null event and the whole sample space. From inequality (7.9) it is immediately evident that $\Pr(T < \infty) = 1$.

With these preliminaries out of the way, we now turn to proving convergence based on a standard coupling argument [134, 169].

Proposition 7.4.1 *Every finite-state ergodic Markov chain has a unique equilibrium distribution* π. *Furthermore, the* n*-step transition probabilities* $p_{ij}^{(n)}$ *satisfy* $\lim_{n \to \infty} p_{ij}^{(n)} = \pi_j$.

Proof: Without loss of generality, we identify the states of the chain with the integers $\{1, \ldots, m\}$. From the inequality

$$\begin{aligned} p_{ij}^{(n)} &= \sum_k p_{ik} p_{kj}^{(n-1)} \\ &\leq \max_l p_{lj}^{(n-1)} \sum_k p_{ik} \\ &= \max_l p_{lj}^{(n-1)} \end{aligned}$$

involving the n-step transition probabilities, we immediately deduce that $\max_i p_{ij}^{(n)}$ is decreasing in n. Likewise, $\min_i p_{ij}^{(n)}$ is increasing in n. If

$$\lim_{n\to\infty} |p_{uj}^{(n)} - p_{vj}^{(n)}| = 0$$

for all initial states u and v, then the gap between $\lim_{n\to\infty} \min_i p_{ij}^{(n)}$ and $\lim_{n\to\infty} \max_i p_{ij}^{(n)}$ is 0. This forces the existence of $\lim_{n\to\infty} p_{ij}^{(n)} = \pi_j$, which we identify as the equilibrium distribution of the chain.

We now construct two coupled chains X_n and Y_n on $\{1, \ldots, m\}$ that individually move according to the transition matrix $P = (p_{ij})$. The X chain starts at u and the Y chain at $v \neq u$. These two chains move independently until the first epoch $T = n$ at which $X_n = Y_n$. Thereafter, they move together. The pair of coupled chains has joint transition matrix

$$p_{(ij),(kl)} = \begin{cases} p_{ik} p_{jl} & \text{if } i \neq j \\ p_{ik} & \text{if } i = j \text{ and } k = l \\ 0 & \text{if } i = j \text{ and } k \neq l\,. \end{cases}$$

By definition it is clear that the probability that the coupled chains occupy the same state at epoch r is at least as great as the probability that two completely independent chains occupy the same state at epoch r. Invoking the ergodic assumption and choosing r so that some power P^r has all of its entries bounded below by a positive constant ϵ, it follows that

$$\Pr(T \leq r \mid X_0 = u, Y_0 = v) \geq \sum_k p_{uk}^{(r)} p_{vk}^{(r)} \geq \epsilon \sum_k p_{vk}^{(r)} = \epsilon.$$

Exactly the same reasoning demonstrates that at every rth epoch the two chains have a chance of colliding of at least ϵ, regardless of their starting positions r epochs previous. In other words, inequality (7.8) holds.

Because $\Pr(T > n)$ is decreasing in n, we now harvest the bound

$$\Pr(T > n) \leq (1-\epsilon)^{\lfloor \frac{n}{r} \rfloor}$$

from inequality (7.9). Combining this bound with the coupling inequality (7.7) yields

$$\frac{1}{2} \sum_j |p_{uj}^{(n)} - p_{vj}^{(n)}| = \|\pi_{X_n} - \pi_{Y_n}\|_{\mathrm{TV}}$$

$$\begin{aligned} &\leq \Pr(X_n \neq Y_n) \\ &\leq \Pr(T > n) \qquad (7.10) \\ &\leq (1-\epsilon)^{\lfloor \frac{n}{r} \rfloor}. \end{aligned}$$

In view of the fact that u and v are arbitrary, this concludes the proof that the $\lim_{n\to\infty} p_{ij}^{(n)} = \pi_j$ exists. ■

In the next example, we concoct a different kind of stopping time $T < \infty$ connected with a Markov chain X_n. If at epoch T the chain achieves its equilibrium distribution π and X_T is independent of T, then T is said to be a strong stationary time. When a strong stationary time exists, it gives considerable insight into the rate of convergence of the underlying chain [3, 49]. In view of the fact that X_n is at equilibrium when $T \leq n$, we readily deduce the total variation bound

$$\|\pi_{X_n} - \pi\|_{\mathrm{TV}} \quad \leq \quad \Pr(T > n). \qquad (7.11)$$

Example 7.4.3 *A Strong Stationary Time for Top-in Shuffling*

In top-in card shuffling, let $T-1$ be the epoch at which the original bottom card reaches the top of the deck. At epoch T the bottom card is reinserted, and the deck achieves equilibrium. For our purposes it is fruitful to view T as the sum $T = S_1 + S_2 + \cdots + S_m$ of independent geometrically distributed random variables. If $T_0 = 0$ and T_i is the first epoch at which i total cards occur under the bottom card, then the waiting time $S_i = T_i - T_{i-1}$ is geometrically distributed with success probability $\frac{i}{m}$. Because $\mathrm{E}(S_i) = \frac{m}{i}$, the strong stationary time T has mean

$$\mathrm{E}(T) \quad = \quad \sum_{i=1}^{m} \frac{m}{i} \quad \approx \quad m \ln m.$$

To exploit the bound (7.11), we consider a random variable T^* having the same distribution as T but generated by a different mechanism. Suppose we randomly drop balls into m equally likely boxes. If we let T^* be the first trial at which no box is empty, then it is clear that we can decompose $T^* = S_m^* + S_{m-1}^* + \cdots + S_1^*$, where S_i^* is the number of trials necessary to go from i empty boxes to $i-1$ empty boxes. Once again the S_i^* are independent and geometrically distributed. This perspective makes it simple to bound $\Pr(T > n)$. Indeed, if A_i is the event that box i is empty after n trials, then

$$\begin{aligned} \Pr(T > n) &= \Pr(T^* > n) \\ &\leq \sum_{i=1}^{m} \Pr(A_i) \\ &= m\left(1 - \frac{1}{m}\right)^n \qquad (7.12) \\ &\leq m e^{-\frac{n}{m}}. \end{aligned}$$

Here we invoke the inequality $\ln(1-x) \leq -x$ for $x \in [0,1)$.

Returning to the top-in shuffle problem, we now combine inequality (7.12) with inequality (7.11). If $n = (1+\epsilon)m \ln m$, we deduce that

$$\|\pi_{X_n} - \pi\|_{\mathrm{TV}} \leq me^{-\frac{(1+\epsilon)m\ln m}{m}} = \frac{1}{m^{\epsilon}},$$

where π is the uniform distribution on permutations of $\{1, \ldots, m\}$. This shows that if we wait much beyond the mean of T, then top-in shuffling will completely randomize the deck. Hence, the mean $\mathrm{E}(T) \approx m \ln m$ serves as a fairly sharp cutoff for equilibrium. Some statistical applications of these ideas appear in reference [131]. ■

7.5 Convergence Rates for Reversible Chains

Although Proposition 7.4.1 proves convergence to equilibrium, it does not provide the best bounds on the rate of convergence. Example 7.4.3 is instructive because it constructs a better and more natural bound. Unfortunately, it is often impossible to identify a strong stationary time. The best estimates of the rate of convergence rely on understanding the eigenstructure of the transition probability matrix P [49, 169]. We now discuss this approach for a reversible ergodic chain with equilibrium distribution π. The inner products

$$\langle u, v\rangle_{1/\pi} = \sum_i \frac{1}{\pi_i} u_i v_i, \qquad \langle u, v\rangle_{\pi} = \sum_i \pi_i u_i v_i$$

feature prominently in our discussion.

For the chain in question, detailed balance translates into the condition

$$\sqrt{\pi_i} p_{ij} \frac{1}{\sqrt{\pi_j}} = \sqrt{\pi_j} p_{ji} \frac{1}{\sqrt{\pi_i}}. \tag{7.13}$$

If D is the diagonal matrix with ith diagonal entry $\sqrt{\pi_i}$, then the validity of equation (7.13) for all pairs (i,j) is equivalent to the symmetry of the matrix $Q = DPD^{-1}$. Let $Q = U\Lambda U^t$ be its spectral decomposition, where U is orthogonal, and Λ is diagonal with ith diagonal entry λ_i. One can rewrite the spectral decomposition as the sum of outer products

$$Q = \sum_i \lambda_i u^i (u^i)^t$$

using the columns u^i of U. The formulas $(u^i)^t u^j = 1_{\{i=j\}}$ and

$$Q^k = \sum_i \lambda_i^k u^i (u^i)^t$$

follow immediately. The formula for Q^k in turn implies

$$P^k = \sum_i \lambda_i^k D^{-1} u^i (u^i)^t D = \sum_i \lambda_i^k w^i v^i, \tag{7.14}$$

where $v^i = (u^i)^t D$ and $w^i = D^{-1} u^i$.

Rearranging the identity $DPD^{-1} = Q = U\Lambda U^t$ yields $U^t DP = \Lambda U^t D$. Hence, the rows v^i of $V = U^t D$ are row eigenvectors of P. These vectors satisfy the orthogonality relations

$$\langle v^i, v^j \rangle_{1/\pi} = v^i D^{-2} (v^j)^t = (u^i)^t u^j = 1_{\{i=j\}}$$

and therefore form a basis of the inner product space $\ell^2_{1/\pi}$. The identity $PD^{-1}U = D^{-1}U\Lambda$ shows that the columns w^j of $W = D^{-1}U$ are column eigenvectors of P. These dual vectors satisfy the orthogonality relations

$$\langle w^i, w^j \rangle_{\pi} = (w^i)^t D^2 w^j = (u^i)^t u^j = 1_{\{i=j\}}$$

and therefore form a basis of the inner product space ℓ^2_π. Finally, we have the biorthogonality relations

$$v^i w^j = 1_{\{i=j\}}$$

under the ordinary inner product. The trivial rescalings $w^i = D^{-2}(v^i)^t$ and $(v^i)^t = D^2 w^i$ allow one to pass back and forth between row eigenvectors and column eigenvectors.

The distance from equilibrium in the $\ell^2_{1/\pi}$ norm bounds the total variation distance from equilibrium in the sense that

$$\|\mu - \pi\|_{\mathrm{TV}} \le \frac{1}{2}\|\mu - \pi\|_{1/\pi}. \tag{7.15}$$

Problem 34 asks for a proof of this fact. With the understanding that $\lambda_1 = 1$, $v^1 = \pi$, and $w^1 = \mathbf{1}$, the next proposition provides an even more basic bound.

Proposition 7.5.1 *An initial distribution μ for a reversible ergodic chain with m states satisfies*

$$\begin{aligned} \|\mu P^k - \pi\|^2_{1/\pi} &= \sum_{i=2}^m \lambda_i^{2k} [(\mu - \pi) w^i]^2 & (7.16) \\ &\le \rho^{2k} \|\mu - \pi\|^2_{1/\pi}, & (7.17) \end{aligned}$$

where $\rho < 1$ is the absolute value of the second-largest eigenvalue in magnitude of the transition probability matrix P.

Proof: Proposition A.2.3 of Appendix A.2 shows that $\rho < 1$. In view of the identity $\pi P = \pi$, the expansion (7.14) gives

$$\begin{aligned}
\|\mu P^k - \pi\|_{1/\pi}^2 &= \|(\mu - \pi)P^k\|_{1/\pi}^2 \\
&= (\mu - \pi)\sum_{i=1}^{m} \lambda_i^k w^i v^i D^{-2} \sum_{j=1}^{m} \lambda_j^k (v^j)^t (w^j)^t (\mu - \pi)^t \\
&= (\mu - \pi)\sum_{i=1}^{m} \lambda_i^{2k} w^i (w^i)^t (\mu - \pi)^t \\
&= \sum_{i=1}^{m} \lambda_i^{2k} \big[(\mu - \pi)w^i\big]^2.
\end{aligned}$$

The two constraints $\sum_j \pi_j = \sum_j \mu_j = 1$ clearly imply $(\mu - \pi)w^1 = 0$. Equality (7.16) follows immediately. Because all remaining eigenvalues satisfy $|\lambda_j| \le \rho$, one can show by similar reasoning that

$$\begin{aligned}
\sum_{j=2}^{m} \lambda_j^{2k} \big[(\mu - \pi)w^i\big]^2 &\le \rho^{2k} \sum_{j=1}^{m} \big[(\mu - \pi)w^i\big]^2 \\
&= \rho^{2k} \|\mu - \pi\|_{1/\pi}^2.
\end{aligned}$$

This validates inequality (7.17). ∎

7.6 Hitting Probabilities and Hitting Times

Consider a Markov chain X_k with state space $\{1, \ldots, n\}$ and transition matrix $P = (p_{ij})$. Suppose that we can divide the states into a transient set $B = \{1, \ldots, m\}$ and an absorbing set $A = \{m + 1, \ldots, n\}$ such that $p_{ij} = 0$ for every $i \in A$ and $j \in B$ and such that every $i \in B$ leads to at least one $j \in A$. Then every realization of the chain starting in B is eventually trapped in A. It is often of interest to find the probability h_{ij} that the chain started at $i \in B$ enters A at $j \in A$. The $m \times (n - m)$ matrix of hitting probabilities $H = (h_{ij})$ can be found by solving the system of equations

$$h_{ij} = p_{ij} + \sum_{k=1}^{m} p_{ik} h_{kj}$$

derived by conditioning on the next state visited by the chain starting from state i. We can summarize this system as the matrix equation $H = R + QH$ by decomposing P into the block matrix

$$P = \begin{pmatrix} Q & R \\ \mathbf{0} & S \end{pmatrix},$$

where Q is $m \times m$, R is $m \times (n-m)$, and S is $(n-m) \times (n-m)$. If I is the $m \times m$ identity matrix, then the formal solution of our system of equations is $H = (I-Q)^{-1}R$. To prove that the indicated matrix inverse exists, we turn to a simple proposition.

Proposition 7.6.1 *Suppose that* $\lim_{k\to\infty} Q^k = \mathbf{0}$, *where* $\mathbf{0}$ *is the* $m \times m$ *zero matrix. Then* $(I-Q)^{-1}$ *exists and equals* $\lim_{l\to\infty} \sum_{k=0}^{l} Q^k$.

Proof: By assumption $\lim_{k\to\infty}(I - Q^k) = I$. Because the determinant function is continuous and $\det I = 1$, it follows that $\det(I - Q^k) \neq 0$ for k sufficiently large. Taking determinants in the identity

$$(I-Q)(I+Q+\cdots+Q^{k-1}) \quad = \quad I - Q^k$$

yields

$$\det(I-Q)\det(I+Q+\cdots+Q^{k-1}) \quad = \quad \det(I-Q^k).$$

Thus, $\det(I-Q) \neq 0$, and $I-Q$ is nonsingular. Finally, the power series expansion for $I-Q$ follows from taking limits in

$$I+Q+\cdots+Q^{k-1} \quad = \quad (I-Q)^{-1}(I-Q^k).$$

This completes the proof. ∎

To apply Proposition 7.6.1, we need to interpret the entries of the matrix $Q^k = (q_{ij}^{(k)})$. A moment's reflection shows that

$$q_{ij}^{(k)} \quad = \quad \sum_{l=1}^{m} q_{il}^{(k-1)} p_{lj}$$

is just the probability that the chain passes from i to j in k steps. Note that the sum defining $q_{ij}^{(k)}$ stops at $l = m$ because once the chain leaves the transient states, it can never reenter them. This fact also makes it intuitively obvious that $\lim_{k\to\infty} q_{ij}^{(k)} = 0$. To verify this limit, it suffices to prove that the chain leaves the transient states after a finite number of steps. Suppose on the contrary that the chain wanders from transient state to transient state forever. In this case, the chain visits some transient state i an infinite number of times. However, i leads to an absorbing state $j > m$ along a path of positive probability. One of these visits to i must successfully take the path to j. This argument can be tightened by defining a first passage time T to the transient states and invoking inequalities (7.8) and (7.9).

In much the same way that we calculate hitting probabilities, we can calculate the mean number of epochs t_{ij} that the chain spends in transient state j prior to absorption starting from transient state i. These expectations satisfy the system of equations

$$t_{ij} \quad = \quad 1_{\{j=i\}} + \sum_{k=1}^{m} p_{ik} t_{kj},$$

which reads as $T = I + QT$ in matrix form. The solution $T = (I - Q)^{-1}$ can be used to write the mean hitting time vector t with ith entry $t_i = \sum_j t_{ij}$ as $t = (I - Q)^{-1}\mathbf{1}$, where $\mathbf{1}$ is the vector with all entries 1. Finally, if f_{ij} is the probability of ever reaching transient state j starting from transient state i, we can rearrange the identity $t_{ij} = f_{ij} t_{jj}$ for $i \neq j$ to yield the simple formula $f_{ij} = t_{ij}/t_{jj}$ for f_{ij}. The analogous identity $t_{ii} = 1 + f_{ii} t_{ii}$ gives $f_{ii} = (t_{ii} - 1)/t_{ii}$.

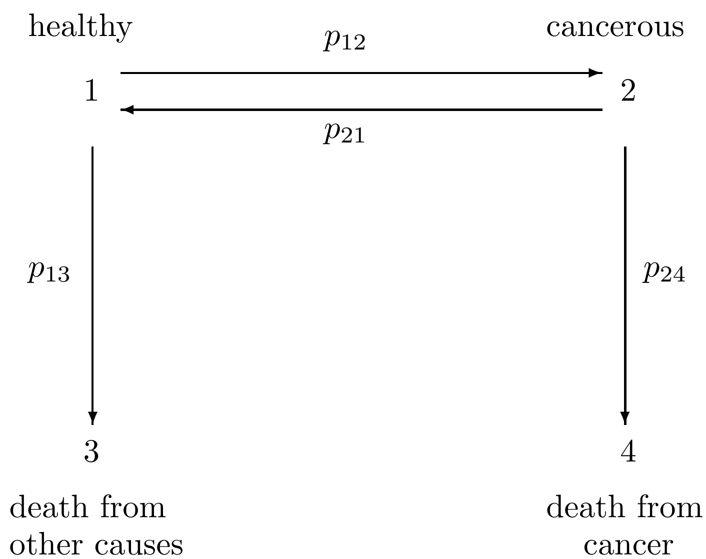

FIGURE 7.1. An Illness-Death Markov Chain

Example 7.6.1 *An Illness-Death Cancer Model*

Figure 7.1 depicts a naive Markov chain model for cancer morbidity and mortality [62]. The two transient states 1 (healthy) and 2 (cancerous) lead to the absorbing states 3 (death from other causes) and 4 (death from cancer). A brief calculation shows that

$$Q = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix}, \qquad R = \begin{pmatrix} p_{13} & 0 \\ 0 & p_{24} \end{pmatrix},$$

and

$$(I - Q)^{-1} = \frac{1}{(1 - p_{11})(1 - p_{22}) - p_{12}p_{21}} \begin{pmatrix} 1 - p_{22} & p_{12} \\ p_{21} & 1 - p_{11} \end{pmatrix}.$$

These are precisely the ingredients necessary to calculate the hitting probabilities $H = (I - Q)^{-1}R$ and mean hitting times $t = (I - Q)^{-1}\mathbf{1}$. ■

7.7 Markov Chain Monte Carlo

The Markov chain Monte Carlo (MCMC) revolution sweeping statistics is drastically changing how statisticians perform integration and summation. In particular, the Metropolis algorithm and Gibbs sampling make it straightforward to construct a Markov chain that samples from a complicated conditional distribution. Once a sample is available, then according to the ergodic theorem, any conditional expectation can be approximated by forming its corresponding sample average. The implications of this insight are profound for both classical and Bayesian statistics. As a bonus, trivial changes to the Metropolis algorithm yield simulated annealing, a general-purpose algorithm for solving difficult combinatorial optimization problems.

Our limited goal in this section is to introduce a few of the major MCMC themes. One issue of paramount importance is how rapidly the underlying chains reach equilibrium. This is the Achilles heel of the whole business and not just a mathematical nicety. Unfortunately, probing this delicate issue is scarcely possible in the confines of a brief overview. We analyze one example to give a feel for the power of coupling and spectral arguments. Readers interested in further pursuing MCMC methods and the related method of simulated annealing will enjoy the pioneering articles [69, 71, 85, 115, 142], the elementary surveys [35, 37], and the books [70, 73, 194].

7.7.1 The Hastings-Metropolis Algorithm

The Hastings-Metropolis algorithm is a device for constructing a Markov chain with a prescribed equilibrium distribution π on a given state space [85, 142]. Each step of the chain is broken into two stages, a proposal stage and an acceptance stage. If the chain is currently in state i, then in the proposal stage a new destination state j is proposed according to a probability density $q_{ij} = q(j \mid i)$. In the subsequent acceptance stage, a random number is drawn uniformly from $[0, 1]$ to determine whether the proposed step is actually taken. If this number is less than the Hastings-Metropolis acceptance probability

$$a_{ij} = \min\left\{\frac{\pi_j q_{ji}}{\pi_i q_{ij}}, 1\right\}, \tag{7.18}$$

then the proposed step is taken. Otherwise, the proposed step is declined, and the chain remains in place. Problem 41 indicates that equation (7.18) defines the most generous acceptance probability consistent with the given proposal mechanism.

Like most good ideas, the Hastings-Metropolis algorithm has undergone successive stages of abstraction and generalization. For instance, Metropolis et al. [142] considered only symmetric proposal densities with $q_{ij} = q_{ji}$. In this case the acceptance probability reduces to

$$a_{ij} = \min\left\{\frac{\pi_j}{\pi_i}, 1\right\}. \tag{7.19}$$

In this simpler setting it is clear that any proposed destination j with $\pi_j > \pi_i$ is automatically accepted. In applying either formula (7.18) or formula (7.19), it is noteworthy that the π_i need only be known up to a multiplicative constant.

To prove that π is the equilibrium distribution of the chain constructed from the Hastings-Metropolis scheme (7.18), it suffices to check that detailed balance holds. If π puts positive weight on all points of the state space, then we must require the inequalities $q_{ij} > 0$ and $q_{ji} > 0$ to be simultaneously true or simultaneously false if detailed balance is to have any chance of holding. Now suppose without loss of generality that the fraction

$$\frac{\pi_j q_{ji}}{\pi_i q_{ij}} \le 1$$

for some $j \neq i$. Then detailed balance follows immediately from

$$\begin{aligned} \pi_i q_{ij} a_{ij} &= \pi_i q_{ij} \frac{\pi_j q_{ji}}{\pi_i q_{ij}} \\ &= \pi_j q_{ji} \\ &= \pi_j q_{ji} a_{ji}. \end{aligned}$$

Besides checking that π is the equilibrium distribution, we should also be concerned about whether the Hastings-Metropolis chain is irreducible and aperiodic. Aperiodicity is the rule because the acceptance-rejection step allows the chain to remain in place. Problem 42 states a precise result and a counterexample. Irreducibility holds provided the entries of π are positive and the proposal matrix $Q = (q_{ij})$ is irreducible.

Example 7.7.1 *Random Walk on a Subset of the Integers*

Random walk sampling occurs when the proposal density $q_{ij} = q_{j-i}$ for some density q_k. This construction requires that the sample space be closed under subtraction. If $q_k = q_{-k}$, then the Metropolis acceptance probability (7.19) applies. ■

Example 7.7.2 *Independence Sampler*

If the proposal density satisfies $q_{ij} = q_j$, then candidate points are drawn independently of the current point. To achieve quick convergence of the chain, q_i should mimic π_i for most i. This intuition is justified by introducing the importance ratios $w_i = \pi_i / q_i$ and rewriting the acceptance probability (7.18) as

$$a_{ij} = \min\left\{\frac{w_j}{w_i}, 1\right\}. \tag{7.20}$$

It is now obvious that it is difficult to exit any state i with a large importance ratio w_i. ■

7.7.2 Gibbs Sampling

The Gibbs sampler is a special case of the Hastings-Metropolis algorithm for Cartesian product state spaces [69, 71, 73]. Suppose that each sample point $i = (i_1, \ldots, i_m)$ has m components. The Gibbs sampler updates one component of i at a time. If the component is chosen randomly and resampled conditional on the remaining components, then the acceptance probability is 1. To prove this assertion, let i_c be the uniformly chosen component, and denote the remaining components by $i_{-c} = (i_1, \ldots, i_{c-1}, i_{c+1}, \ldots, i_m)$. If j is a neighbor of i reachable by changing only component i_c, then $j_{-c} = i_{-c}$. For such a neighbor j, the proposal probability

$$q_{ij} = \frac{1}{m} \cdot \frac{\pi_j}{\sum_{\{k:k_{-c}=i_{-c}\}} \pi_k}$$

satisfies $\pi_i q_{ij} = \pi_j q_{ji}$, and the ratio appearing in the acceptance probability (7.18) is 1.

In contrast to random sampling of components, we can repeatedly cycle through the components in some fixed order, say $1, 2, \ldots, m$. If the transition matrix for changing component c while leaving other components unaltered is $P^{(c)}$, then the transition matrices for random sampling and sequential (or cyclic) sampling are $R = \frac{1}{m}\sum_c P^{(c)}$ and $S = P^{(1)} \cdots P^{(m)}$, respectively. Because each $P^{(c)}$ satisfies $\pi P^{(c)} = \pi$, we have $\pi R = \pi$ and $\pi S = \pi$ as well. Thus, π is the unique equilibrium distribution for R or S if either is irreducible. However as pointed out in Problem 43, R satisfies detailed balance while S ordinarily does not.

Example 7.7.3 *Ising Model*

Consider m elementary particles equally spaced around the boundary of the unit circle. Each particle c can be in one of two magnetic states—spin up with $i_c = 1$ or spin down with $i_c = -1$. The Gibbs distribution

$$\pi_i \propto e^{\beta \sum_d i_d i_{d+1}} \tag{7.21}$$

takes into account nearest-neighbor interactions in the sense that states like $(1, 1, 1, \ldots, 1, 1, 1)$ are favored and states like $(1, -1, 1, \ldots, 1, -1, 1)$ are shunned for $\beta > 0$. (Note that in equation (7.21) the index $m + 1$ of i_{m+1} is interpreted as 1.) There is no need to specify the normalizing constant (or partition function)

$$Z = \sum_i e^{\beta \sum_d i_d i_{d+1}}$$

to carry out Gibbs sampling. If we elect to resample component c, then the choices $j_c = -i_c$ and $j_c = i_c$ are made with respective probabilities

$$\begin{aligned}
\frac{e^{\beta(-i_{c-1}i_c - i_c i_{c+1})}}{e^{\beta(i_{c-1}i_c + i_c i_{c+1})} + e^{\beta(-i_{c-1}i_c - i_c i_{c+1})}} &= \frac{1}{e^{2\beta(i_{c-1}i_c + i_c i_{c+1})} + 1} \\
\frac{e^{\beta(i_{c-1}i_c + i_c i_{c+1})}}{e^{\beta(i_{c-1}i_c + i_c i_{c+1})} + e^{\beta(-i_{c-1}i_c - i_c i_{c+1})}} &= \frac{1}{1 + e^{-2\beta(i_{c-1}i_c + i_c i_{c+1})}}.
\end{aligned}$$

When the number of particles m is even, the odd-numbered particles are independent given the even-numbered particles, and vice versa. This fact suggests alternating between resampling all odd-numbered particles and resampling all even-numbered particles. Such multi-particle updates take longer to execute but create more radical rearrangements than single-particle updates. ■

7.7.3 Convergence of the Independence Sampler

For the independence sampler, it is possible to give a coupling bound on the rate of convergence to equilibrium [137]. Suppose that $X_0, X_1, \ldots$ represents the sequence of states visited by the independence sampler starting from $X_0 = x_0$. We couple this Markov chain to a second independence sampler $Y_0, Y_1, \ldots$ starting from the equilibrium distribution π. By definition, each Y_k has distribution π. The two chains are coupled by a common proposal stage and a common uniform deviate U sampled in deciding whether to accept the common proposed point. They differ in having different acceptance probabilities. If $X_n = Y_n$ for some n, then $X_k = Y_k$ for all $k \geq n$. Let T denote the random epoch when X_n first meets Y_n and the X chain attains equilibrium.

The importance ratios $w_j = \pi_j / q_j$ determine what proposed points are accepted. Without loss of generality, assume that the states of the chain are numbered $1, \ldots, m$ and that the importance ratios w_i are in decreasing order. If $X_n = x \neq y = Y_n$, then according to equation (7.18) the next proposed point is accepted by both chains with probability

$$\begin{aligned}
\sum_{j=1}^{m} q_j \min\left\{\frac{w_j}{w_x}, \frac{w_j}{w_y}, 1\right\} &= \sum_{j=1}^{m} \pi_j \min\left\{\frac{1}{w_x}, \frac{1}{w_y}, \frac{1}{w_j}\right\} \\
&\geq \frac{1}{w_1}.
\end{aligned}$$

In other words, at each trial the two chains meet with at least probability $1/w_1$. This translates into the tail probability bound

$$\Pr(T > n) \quad \leq \quad \left(1 - \frac{1}{w_1}\right)^n. \qquad (7.22)$$

By the same type of reasoning that led to inequality (7.10), we deduce the further bound

$$\begin{aligned} \|\pi_{X_n} - \pi\|_{\mathrm{TV}} &\leq \Pr(X_n \neq Y_n) \\ &= \Pr(T > n) \\ &\leq \left(1 - \frac{1}{w_1}\right)^n \end{aligned} \qquad (7.23)$$

on the total variation distance of X_n from equilibrium.

It is interesting to compare this last bound with the bound entailed by Proposition 7.5.1. Based on our assumption that the importance ratios are decreasing, equation (7.20) shows that the transition probabilities of the independence sampler are

$$p_{ij} = \begin{cases} q_j & j < i \\ \pi_j/w_i & j > i\,. \end{cases}$$

In order for $\sum_j p_{ij} = 1$, we must set $p_{ii} = q_i + \lambda_i$, where

$$\lambda_i = \sum_{k=i}^{m}\left(q_k - \frac{\pi_k}{w_i}\right) = \sum_{k=i+1}^{m}\left(q_k - \frac{\pi_k}{w_i}\right).$$

With these formulas in mind, one can decompose the overall transition probability matrix as $P = U + \mathbf{1}q$, where $q = (q_1, \ldots, q_m)$ and U is the upper triangular matrix

$$U = \begin{pmatrix} \lambda_1 & \frac{q_2(w_2-w_1)}{w_1} & \cdots & \cdots & \frac{q_{m-1}(w_{m-1}-w_1)}{w_1} & \frac{q_m(w_m-w_1)}{w_1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_{m-1} & \frac{q_m(w_m-w_{m-1})}{w_{m-1}} \\ 0 & 0 & 0 & \cdots & 0 & \lambda_m \end{pmatrix}.$$

The eigenvalues of U are just its diagonal entries λ_1 through λ_m.

The reader can check that (a) $\lambda_1 = 1 - 1/w_1$, (b) the λ_i are decreasing, and (c) $\lambda_m = 0$. It turns out that P and U share most of their eigenvalues. They differ in the eigenvalue attached to the eigenvector $\mathbf{1}$ since $P\mathbf{1} = \mathbf{1}$ and $U\mathbf{1} = \mathbf{0}$. Suppose $Uv = \lambda_i v$ for some i between 1 and $m-1$. Let us construct a column eigenvector of P with the eigenvalue λ_i. As a trial eigenvector we take $v + c\mathbf{1}$ and calculate

$$(U + \mathbf{1}q)(v + c\mathbf{1}) = \lambda_i v + qv\mathbf{1} + c\mathbf{1} = \lambda_i v + (qv + c)\mathbf{1}.$$

This is consistent with $v + c\mathbf{1}$ being an eigenvector provided we choose the constant c to satisfy $qv + c = \lambda_i c$. Because $\lambda_i \neq 1$, it is always possible to do so. The combination of Proposition 7.5.1 and inequality (7.15) gives a bound that decays at the same geometric rate $\lambda_1 = 1 - w_1^{-1}$ as the coupling bound (7.23). Thus, the coupling bound is about as good as one could hope for. Problems 44 and 45 ask the reader to flesh out our convergence arguments.

7.8 Simulated Annealing

In simulated annealing we are interested in finding the most probable state of a Markov chain [115, 163]. If this state is k, then $\pi_k > \pi_i$ for all $i \neq k$. To accentuate the weight given to state k, we can replace the equilibrium distribution π by a distribution putting probability

$$\pi_i^{(\tau)} = \frac{\pi_i^{1/\tau}}{\sum_j \pi_j^{1/\tau}}$$

on state i. Here τ is a positive parameter traditionally called temperature. With a symmetric proposal density, the distribution $\pi_i^{(\tau)}$ can be attained by running a chain with Metropolis acceptance probability

$$a_{ij} = \min\left\{\left(\frac{\pi_j}{\pi_i}\right)^{1/\tau}, 1\right\}. \tag{7.24}$$

In simulated annealing, the chain is run with τ gradually decreasing to 0 rather than with τ fixed. If τ starts out large, then in the early stages of simulated annealing, almost all proposed steps are accepted, and the chain broadly samples the state space. As τ declines, fewer unfavorable steps are taken, and the chain eventually settles on some nearly optimal state. With luck, this state is k or a state equivalent to k if several states are optimal. Simulated annealing is designed to mimic the gradual freezing of a substance into a crystalline state of perfect symmetry and hence minimum energy.

Example 7.8.1 *The Traveling Salesman Problem*

As discussed in Example 5.7.2, a salesman must visit m towns, starting and ending in his hometown. Given fixed distances d_{ij} between every pair of towns i and j, in what order should he visit the towns to minimize the length of his circuit? This problem belongs to the class of NP-complete problems; these have deterministic solutions that are conjectured to increase in complexity at an exponential rate in m.

In the simulated annealing approach to the traveling salesman problem, we assign to each permutation $\sigma = (\sigma_1, \ldots, \sigma_m)$ a cost $c_\sigma = \sum_{i=1}^m d_{\sigma_i, \sigma_{i+1}}$, where $\sigma_{m+1} = \sigma_1$. Defining $\pi_\sigma \propto e^{-c_\sigma}$ turns the problem of minimizing the cost into one of finding the most probable permutation σ. In the proposal stage of simulated annealing, we randomly select two indices $i < j$ and reverse the block of integers beginning at σ_i and ending at σ_j in the current permutation $(\sigma_1, \ldots, \sigma_m)$. Thus, if $(4, 7, 5, 2, 3, 1, 6)$ is the current permutation and indices 3 and 6 are selected, then the proposed permutation is $(4, 7, 1, 3, 2, 5, 6)$. A proposal is accepted with probability (7.24) depending on the temperature τ. In *Numerical Recipes'* [163] simulated annealing algorithm for the traveling salesman problem, τ is lowered in multiplicative decrements of 10% after every $100m$ epochs or every $10m$ accepted steps, whichever comes first. ■

7.9 Problems

1. Take three numbers x_1, x_2, and x_3 and form the successive running averages $x_n = (x_{n-3} + x_{n-2} + x_{n-1})/3$ starting with x_4. Prove that
$$\lim_{n\to\infty} x_n = \frac{x_1 + 2x_2 + 3x_3}{6}.$$

2. A drunken knight is placed on an empty chess board and randomly moves according to the usual chess rule. Calculate the equilibrium distribution of the knight's position [152]. (Hints: Consider the squares to be nodes of a graph. Connect two squares by an edge if the knight can move from one to the other in one step. Show that the graph is connected and that 4 squares have degree 2, 8 squares have degree 3, 20 squares have degree 4, 16 squares have degree 6, and 16 squares have degree 8.)

3. Suppose you repeatedly throw a fair die and record the sum S_n of the exposed faces after n throws. Show that
$$\lim_{n\to\infty} \Pr(S_n \text{ is divisible by } 13) = \frac{1}{13}$$
by constructing an appropriate Markov chain [152].

4. Demonstrate that a finite-state Markov chain is ergodic (irreducible and aperiodic) if and only if some power P^n of the transition matrix P has all entries positive. (Hints: For sufficiency, show that if some power P^n has all entries positive, then P^{n+1} has all entries positive. For necessity, note that $p_{ij}^{(r+s+t)} \geq p_{ik}^{(r)} p_{kk}^{(s)} p_{kj}^{(t)}$, and use the number theoretic fact that the set $\{s : p_{kk}^{(s)} > 0\}$ contains all sufficiently large positive integers s if k is aperiodic. See Appendix A.1 for the requisite number theory.)

5. Consider the Cartesian product state space $A \times B$, where
$$A = \{0, 1, \ldots, a-1\}, \quad B = \{0, 1, \ldots, b-1\},$$
and a and b are positive integers. Define a Markov chain that moves from (x, y) to $(x+1 \bmod a, y)$ or $(x, y+1 \bmod b)$ with equal probability at each epoch. Show that the chain is irreducible. Also show that it is aperiodic if and only if the greatest common divisor of a and b is 1. (Hints: It helps to consider the special state $(0, 0)$. See Proposition A.1.4 of Appendix A.1.)

6. Prove that every state of an irreducible Markov chain has the same period.

7. Suppose an irreducible Markov chain has period d. Show that the states of the chain can be divided into d disjoint classes $C_0, \ldots, C_{d-1}$ such that $p_{ij} = 0$ unless $i \in C_k$ and $j \in C_l$ for $l = k + 1 \bmod d$. (Hint: Fix a state u and define $C_r = \{v : p_{uv}^{(nd+r)} > 0 \text{ for some } n \geq 0\}$.)

8. The transition matrix P of a finite Markov chain is said to be doubly stochastic if each of its column sums equals 1. Find an equilibrium distribution in this setting. Prove that symmetric transition matrices are doubly stochastic. For a nontrivial example of a doubly stochastic transition matrix, see Example 7.3.5.

9. Demonstrate that an irreducible Markov chain possesses at most one equilibrium distribution. This result applies regardless of whether the chain is finite or aperiodic. (Hints: Let $P = (p_{ij})$ be the transition matrix and π and μ be two different equilibrium distributions. Then there exist two states j and k with $\pi_j > \mu_j$ and $\pi_k < \mu_k$. For some state i choose m and n such that $p_{ji}^{(m)} > 0$ and $p_{ki}^{(n)} > 0$. If we define $Q = \frac{1}{2}P^m + \frac{1}{2}P^n$, then prove that $\pi = \pi Q$ and $\mu = \mu Q$. Furthermore, prove that strict inequality holds in the inequality

$$\begin{aligned} \|\pi - \mu\|_{\mathrm{TV}} &= \frac{1}{2}\sum_i \Big| \sum_l (\pi_l - \mu_l) q_{li} \Big| \\ &\leq \frac{1}{2}\sum_l |\pi_l - \mu_l| \sum_i q_{li} \\ &= \|\pi - \mu\|_{\mathrm{TV}}. \end{aligned}$$

This contradiction gives the desired conclusion. Observe that the proof does not use the full force of irreducibility. The argument is valid for a chain with transient states provided they all can reach the designated state i.)

10. Show that Kolmogorov's criterion (7.3) implies that definition (7.4) does not depend on the particular path chosen from i to j.

11. In the Bernoulli-Laplace model, we imagine two boxes with m particles each. Among the $2m$ particles there are b black particles and w white particles, where $b + w = 2m$ and $b \leq w$. At each epoch one particle is randomly selected from each box, and the two particles are exchanged. Let Z_n be the number of black particles in the first box. Is the corresponding chain irreducible, aperiodic, and/or reversible? Show that its equilibrium distribution is hypergeometric.

12. In Example 7.3.1, show that the chain is aperiodic if and only if the underlying graph is not bipartite.

13. A random walk on a connected graph has equilibrium distribution $\pi_v = \frac{d(v)}{2m}$, where $d(v)$ is the degree of v and m is the number of edges. Let t_{uv} be the expected time the chain takes in traveling from node u to node v. If the graph is not bipartite, then the chain is aperiodic, and Example 7.3.4 shows that $t_{vv} = 1/\pi_v$. Write a recurrence relation connecting t_{vv} to the t_{uv} for nodes u in the neighborhood of v, and use the relation to demonstrate that $t_{uv} \leq 2m - d(v)$ for each such u.

14. Consider the $n!$ different permutations $\sigma = (\sigma_1, \ldots, \sigma_n)$ of the set $\{1, \ldots, n\}$ equipped with the uniform distribution $\pi_\sigma = 1/n!$ [49]. Declare a permutation ω to be a neighbor of σ if there exist two indices $i \neq j$ such that $\omega_i = \sigma_j$, $\omega_j = \sigma_i$, and $\omega_k = \sigma_k$ for $k \notin \{i, j\}$. How many neighbors does a permutation σ possess? Show how the set of permutations can be made into a reversible Markov chain using the construction of Example 7.3.1. Is the underlying graph bipartite? If we execute one step of the chain by randomly choosing two indices i and j and switching σ_i and σ_j, how can we slightly modify the chain so that it is aperiodic?

15. Consider a set of b light bulbs. At epoch n, a random subset of s light bulbs is selected. Those bulbs in the subset that are on are switched off, and those bulbs that are off are switched on. Let X_n equal the total number of on bulbs just after this random event.

    (a) Show that the stochastic process X_n is a Markov chain. What is the state space? (Hint: You may want to revise your answer after considering question (c).)

    (b) Demonstrate that the transition probability matrix has entries

    $$p_{jk} \quad = \quad \Pr(X_{n+1} = k \mid X_n = j) \quad = \quad \frac{\binom{j}{i}\binom{b-j}{s-i}}{\binom{b}{s}}.$$

    where $i = (s + j - k)/2$ must be an integer. Note that $p_{jk} > 0$ if and only if $p_{kj} > 0$.

    (c) Verify the following behavior. If s is an even integer and X_0 is even, then all subsequent X_n are even. If s is an even integer and X_0 is odd, then all subsequent X_n are odd. If s is an odd integer, then the X_n alternate between even and odd values. What is the period of the chain when s is odd? Recall that the period of state i is the greatest common divisor of the set $\{n \geq 1 : p_{ii}^{(n)} > 0\}$, where $p_{ii}^{(n)}$ is an n-step transition probability. If all states communicate, then every state has the same period.

    (d) If s is odd, then prove that all states communicate. If s is even, then prove that all even states communicate and that all odd states communicate. (Hints: First, show that it is possible to pass in a finite number of steps from any state j to some state k with $k \leq s$. Second, show that it suffices to assume $b = s + 1$. Third, consider the paths

$$\begin{array}{c} 0 \leftrightarrow s \leftrightarrow 2 \leftrightarrow s-2 \leftrightarrow 4 \leftrightarrow \cdots \leftrightarrow \lfloor \frac{s}{2} \rfloor \\ s+1 \leftrightarrow 1 \leftrightarrow s-1 \leftrightarrow 3 \leftrightarrow s-3 \leftrightarrow \cdots \leftrightarrow \lfloor \frac{s}{2} \rfloor + 1. \end{array}$$

Every state between 0 and $s + 1$ is visited by one of these two paths. When s is odd, the transition $\lfloor \frac{s}{2} \rfloor \leftrightarrow \lfloor \frac{s}{2} \rfloor + 1$ is possible. If this reasoning is too complicated, show how states communicate for a particular choice of s, say 4 or 5.)

(e) Verify that the unique stationary distribution π of the chain has entries

$$\pi_j = \frac{\binom{b}{j}}{2^b} \quad \text{or} \quad \pi_j = \frac{\binom{b}{j}}{2^{b-1}}.$$

(Hints: Check detailed balance. For the normalizing constant when s is even, suppose that X follows the equilibrium distribution π. If X is concentrated on the even integers, then it has generating function

$$\mathrm{E}(u^X) = \left(\frac{1}{2} + \frac{u}{2}\right)^b + \left(\frac{1}{2} - \frac{u}{2}\right)^b,$$

and if X is concentrated on the odd integers, then it has generating function

$$\mathrm{E}(u^X) = \left(\frac{1}{2} + \frac{u}{2}\right)^b - \left(\frac{1}{2} - \frac{u}{2}\right)^b.$$

Evaluate when $u = 1$.)

(f) Suppose that X follows the equilibrium distribution. Demonstrate that X has mean $\mathrm{E}(X) = \frac{b}{2}$. If s is even and X is concentrated on the even integers, then show that X has falling factorial moments

$$\mathrm{E}[(X)_k] = \begin{cases} \frac{(b)_k}{2^k} & 0 \leq k < b \\ \frac{b!}{2^b}[1 + (-1)^b] & k = b \\ 0 & k > b. \end{cases}$$

If s is even and X is concentrated on the odd integers, these factorial moments become

$$\mathrm{E}[(X)_k] = \begin{cases} \frac{(b)_k}{2^k} & 0 \leq k < b \\ \frac{b!}{2^b}[1 - (-1)^b] & k = b \\ 0 & k > b. \end{cases}$$

Let Y be binomially distributed with b trials and success probability $\frac{1}{2}$. It is interesting that $\mathrm{E}[(X)_k] = \mathrm{E}[(Y)_k]$ for $k < b$. This fact implies that X and Y have the same ordinary moments $\mathrm{E}(X^k) = \mathrm{E}(Y^k)$ for $k < b$. (Hint: See the hint to the last subproblem.)

16. In Example 7.4.1, suppose that $f(x)$ is strictly increasing and $g(x)$ is increasing. Show that $\mathrm{Cov}[f(X), g(X)] = 0$ occurs if and only if $\Pr[g(X) = c] = 1$ for some constant c. (Hint: For necessity, examine the proof of the example and show that $\mathrm{Cov}[f(X), g(X)] = 0$ entails $\Pr[g(X) = g(Y)] = 1$ and therefore $\mathrm{Var}[g(X) - g(Y)] = 0$.)

17. Consider a random graph with n nodes. Between every pair of nodes, independently introduce an edge with probability p. If $c(p)$ denotes the probability that the graph is connected, then it is intuitively clear that $c(p)$ is increasing in p. Give a coupling proof of this fact.

18. Consider a random walk on the integers $0, \ldots, m$ with transition probabilities

$$p_{ij} = \begin{cases} q_i & j = i - 1 \\ 1 - q_i & j = i + 1 \end{cases}$$

for $i = 1, \ldots, m - 1$ and $p_{00} = p_{mm} = 1$. All other transition probabilities are 0. Eventually the walk gets trapped at 0 or m. Let f_i be the probability that the walk is absorbed at 0 starting from i. Show that f_i is an increasing function of the entries of $q = (q_1, \ldots, q_{m-1})$. (Hint: Let q and q^* satisfy $q_i \leq q_i^*$ for $i = 1, \ldots, m - 1$. Construct coupled walks X_n and Y_n based on q and q^* such that $X_0 = Y_0 = i$ and such that at the first step $Y_1 \leq X_1$. This requires coordinating the first step of each chain. If $X_1 > Y_1$, then run the X_n chain until it reaches either m or Y_1. In the latter case, take another coordinated step of the two chains.)

19. Suppose that X follows the hypergeometric distribution

$$\Pr(X = i) = \frac{\binom{r}{i}\binom{n-r}{m-i}}{\binom{n}{m}}.$$

Let Y follow the same hypergeometric distribution except that $r + 1$ replaces r. Give a coupling proof that $\Pr(X \geq k) \leq \Pr(Y \geq k)$ for all k. (Hint: Consider an urn with r red balls, 1 white ball, and $n - r - 1$ black balls. If we draw m balls from the urn without replacement, then X is the number of red balls drawn, and Y is the number of red or white balls drawn.)

20. Let X be a binomially distributed random variable with n trials and success probability p. Show by a coupling argument that $\Pr(X \geq k)$ is increasing in n for fixed p and k and in p for fixed n and k.

21. Let Y be a Poisson random variable with mean λ. Demonstrate that $\Pr(Y \geq k)$ is increasing in λ for k fixed. (Hint: If $\lambda_1 < \lambda_2$, then construct coupled Poisson random variables Y_1 and Y_2 with means λ_1 and λ_2 such that $Y_1 \leq Y_2$.)

22. Let Y follow a negative binomial distribution that counts the number of failures until n successes. Demonstrate by a coupling argument that $\Pr(Y \geq k)$ is decreasing in the success probability p for k fixed.

23. Let X_1 follow a beta distribution with parameters α_1 and β_1 and X_2 follow a beta distribution with parameters α_2 and β_2. If $\alpha_1 \leq \alpha_2$ and $\alpha_1 + \beta_1 = \alpha_2 + \beta_2$, then demonstrate that $\Pr(X_1 \geq x) \leq \Pr(X_2 \geq x)$ for all $x \in [0, 1]$. How does this result carry over to the beta-binomial distribution? (Hint: Construct X_1 and X_2 from gamma distributed random variables.)

24. The random variable Y stochastically dominates the random variable X provided $\Pr(Y \leq u) \leq \Pr(X \leq u)$ for all real u. Using quantile coupling, we can construct on a common probability space probabilistic copies X_c of X and Y_c of Y such that $X_c \leq Y_c$ with probability 1. If X has distribution function $F(x)$ and Y has distribution function $G(y)$, then define $F^{[-1]}(u)$ and $G^{[-1]}(u)$ as instructed in Example 1.5.1 of Chapter 1. If U is uniformly distributed on $[0, 1]$, demonstrate that $X_c = F^{[-1]}(U)$ and $Y_c = G^{[-1]}(U)$ yield quantile couplings with the property $X_c \leq Y_c$. Problems 19 through 23 provide examples of stochastic domination.

25. Continuing Problem 24, suppose that X_1, X_2, Y_1, and Y_2 are random variables such that Y_1 dominates X_1, Y_2 dominates X_2, X_1 and X_2 are independent, and Y_1 and Y_2 are independent. Prove that $Y_1 + Y_2$ dominates $X_1 + X_2$.

26. Suppose that the random variable Y stochastically dominates the random variable X and that $f(u)$ is an increasing function of the real variable u. In view of Problem 24, prove that

$$\mathrm{E}[f(Y)] \quad \geq \quad \mathrm{E}[f(X)]$$

whenever both expectations exist. Conversely, if X and Y have this property, then show that Y stochastically dominates X.

27. Suppose the integer-valued random variable Y stochastically dominates the integer-valued random variable X. Prove the bound

$$\|\pi_X - \pi_Y\|_{\mathrm{TV}} \quad \leq \quad \mathrm{E}(Y) - \mathrm{E}(X)$$

by extending inequality (7.7). Explicitly evaluate this bound for the distributions featured in Problems 19 through 23. (Hint: According to Problem 24, one can assume that $Y \geq X$.)

28. Show that the two definitions of the total variation norm given in equation (7.6) coincide.

29. Let X have a Bernoulli distribution with success probability p and Y a Poisson distribution with mean p. Prove the total variation inequality

$$\|\pi_X - \pi_Y\|_{\mathrm{TV}} \quad \leq \quad p^2 \tag{7.25}$$

involving the distributions π_X and π_Y of X and Y.

30. Suppose the integer-valued random variables U_1, U_2, V_1, and V_2 are such that U_1 and U_2 are independent and V_1 and V_2 are independent. Demonstrate that

$$\|\pi_{U_1+U_2} - \pi_{V_1+V_2}\|_{\mathrm{TV}} \;\leq\; \|\pi_{U_1} - \pi_{V_1}\|_{\mathrm{TV}} + \|\pi_{U_2} - \pi_{V_2}\|_{\mathrm{TV}}. \tag{7.26}$$

31. A simple change of Ehrenfest's Markov chain in Example 7.3.3 renders it ergodic. At each step of the chain, flip a fair coin. If the coin lands heads, switch the chosen molecule to the other half of the box. If the coin lands tails, leave it where it is. Show that Ehrenfest's chain with holding is ergodic and converges to the binomial distribution π with m trials and success probability $\frac{1}{2}$. The rate of convergence to this equilibrium distribution can be understood by constructing a strong stationary time. As each molecule is encountered, check it off the list of molecules. Let T be the first time all m molecules are checked off. Argue that T is a strong stationary time. If $\pi^{(n)}$ is the state of the chain at epoch n, then also show that

$$\|\pi^{(n)} - \pi\|_{\mathrm{TV}} \quad \leq \quad m\Big(1 - \frac{1}{m}\Big)^n$$

and therefore that

$$\|\pi^{(n)} - \pi\|_{\mathrm{TV}} \quad \leq \quad e^{-c}$$

for $n = m \ln m + cm$ and $c > 0$.

32. Suppose in the Wright-Fisher model of Example 7.3.2 that each sampled a_1 allele has a chance of u of mutating to an a_2 allele and that each sampled a_2 allele has a chance of v of mutating to an a_1 allele, where the mutation rates u and v are taken from $(0, 1)$. If the number Z_n of a_1 alleles at generation n equals i, then show that Z_{n+1} is binomially distributed with success probability

$$p_i \quad = \quad \frac{i}{2m}(1-u) + \frac{2m-i}{2m}v.$$

Also prove:

(a) The p_i are increasing in i provided $u+v \leq 1$.

(b) The chain is ergodic.

(c) When $u+v=1$, the chain is reversible with equilibrium distribution

$$\pi_j = \binom{2m}{j} v^j u^{2m-j}.$$

(d) When $u+v \neq 1$, the chain can be irreversible. For a counterexample, choose $m=1$ and consider the path $0 \to 1 \to 2 \to 0$ and its reverse. Show that the circulation criterion can fail.

Although it is unclear what the equilibrium distribution is in general, Hua Zhou has constructed a coupling that bounds the rate of convergence of the chain to equilibrium. Assume that $u+v<1$ and fix any two initial states $x<y$ in $\{0,1,\ldots,2m\}$. Let X_n be a realization of the chain starting from x and Y_n be a realization of the chain starting from y. We couple the chains by coordinated sampling of the $2m$ replacement genes at each generation. For the kth sampled gene in forming generation $n+1$, let U_k be a uniform deviate from $(0,1)$. If $U_k \leq p_{X_n}$, then declare the gene to be an a_1 allele in the X process. If $U_k \leq p_{Y_n}$, then declare the gene to be an a_1 allele in the Y process. Why does this imply that $X_{n+1} \leq Y_{n+1}$? Once $X_n = Y_n$ for some n, they stay coupled. In view of Problem 27, supply the reasons behind the following string of equalities and inequalities:

$$\begin{aligned}
\|\pi_{X_n} - \pi_{Y_n}\|_{\mathrm{TV}} &\leq \mathrm{E}(Y_n - X_n) \\
&= (1-u-v)\,\mathrm{E}(Y_{n-1} - X_{n-1}) \\
&= (1-u-v)^n (y-x) \\
&\leq 2m(1-u-v)^n.
\end{aligned}$$

Since x and y are arbitrary, this implies that the mixing time for the chain is on the order of $O\left(\frac{\ln(2m)}{u+v}\right)$ generations.

33. As another example of a strong uniform time, consider the inverse shuffling method of Reeds [49]. At every shuffle we imagine that each of c cards is assigned independently and uniformly to a top pile or a bottom pile. Hence, each pile has a binomial number of cards with mean $\frac{c}{2}$. The order of the two subpiles is kept consistent with the order of the parent pile, and in preparation for the next shuffle, the top pile is placed above the bottom pile. To keep track of the process, one can mark each card with a 0 (top pile) or 1 (bottom pile). Thus, shuffling induces an infinite binary sequence on each card that serves to track its fate. Let T denote the epoch when the first n digits for each card are unique. At T the cards reach a completely random

state where all c permutations are equally likely. Let π be the uniform distribution and π_{X_n} be the distribution of the cards after n shuffles. The probability $\Pr(T \le n)$ is the same as the probability that c balls (digit strings) dropped independently and uniformly into 2^n boxes all wind up in different boxes. With this background in mind, deduce the bound

$$\|\pi_{X_n} - \pi\|_{\mathrm{TV}} \quad \le \quad 1 - \prod_{i=1}^{c-1}\Big(1 - \frac{i}{2^n}\Big).$$

Plot or tabulate the bound as a function of n for $c = 52$ cards. How many shuffles guarantee randomness with high probability?

34. Prove inequality (7.15) by applying the Cauchy-Schwarz inequality. Also verify that P satisfies the self-adjointness condition

$$\langle Pu, v\rangle_\pi \quad = \quad \langle u, Pv\rangle_\pi,$$

which yields a direct proof that P has only real eigenvalues.

35. Let $Z_0, Z_1, Z_2, \ldots$ be a realization of a finite-state ergodic chain. If we sample every kth epoch, then show (a) that the sampled chain $Z_0, Z_k, Z_{2k}, \ldots$ is ergodic, (b) that it possesses the same equilibrium distribution as the original chain, and (c) that it is reversible if the original chain is. Thus, based on the ergodic theorem, we can estimate theoretical means by sample averages using only every kth epoch of the original chain.

36. Consider the symmetric random walk S_n with

$$\Pr(S_{n+1} = S_n + 1) \quad = \quad \Pr(S_{n+1} = S_n - 1) \quad = \quad \frac{1}{2}.$$

Given $S_0 = i \ne 0$, let π_i be the probability that the random walk eventually hits 0. Show that

$$\begin{aligned} \pi_1 &= \frac{1}{2} + \frac{1}{2}\pi_2 \\ \pi_k &= \pi_1^k, \quad k > 0. \end{aligned}$$

Use these two equations to prove that all $\pi_i = 1$. (Hint: Symmetry.)

37. Continuing Problem 36, let μ_k be the expected waiting time for a first passage from k to 0. Show that $\mu_k = k\mu_1$ and that

$$\mu_k \quad = \quad 1 + \frac{1}{2}\mu_{k-1} + \frac{1}{2}\mu_{k+1}$$

for $k \ge 2$. Conclude from these identities that $\mu_k = \infty$ for all $k \ge 1$. Now reason that $\mu_0 = 1 + \mu_1$ and deduce that $\mu_0 = \infty$ as well.

38. Consider a random walk on the integers $\{0, 1, \ldots, n\}$. States 0 and n are absorbing in the sense that $p_{00} = p_{nn} = 1$. If i is a transient state, then the transition probabilities are $p_{i,i+1} = p$ and $p_{i,i-1} = q$, where $p + q = 1$. Verify that the hitting probabilities are

$$h_{in} = 1 - h_{i0} = \begin{cases} \frac{(\frac{q}{p})^i - 1}{(\frac{q}{p})^n - 1}, & p \neq q \\ \frac{i}{n}, & p = q \end{cases}$$

and the mean hitting times are

$$t_i = \begin{cases} \frac{n}{p-q} \frac{(\frac{q}{p})^i - 1}{(\frac{q}{p})^n - 1} - \frac{i}{p-q}, & p \neq q \\ i(n-i), & p = q. \end{cases}$$

(Hint: First argue that

$$t_i = 1 + \sum_{k=1}^{m} p_{ik} t_k$$

in the notation of Section 7.6.)

39. Arrange n points labeled $0, \ldots, n-1$ symmetrically on a circle, and imagine conducting a symmetric random walk with transition probabilities

$$p_{ij} = \begin{cases} \frac{1}{2} & j = i + 1 \bmod n \text{ or } j = i - 1 \bmod n \\ 0 & \text{otherwise}. \end{cases}$$

Thus, only transitions to nearest neighbors are allowed. Let e_k be the expected number of epochs until reaching point 0 starting at point k. Interpret e_0 as the expected number of epochs to return to 0. In finding the e_k, argue that it suffices to find $e_0, \ldots, e_m$, where $m = \lfloor \frac{n}{2} \rfloor$. Write a system of recurrence relations for the e_k, and show that the system has the solution

$$e_k = \begin{cases} n & k = 0 \\ k(n-k) & 1 \leq k \leq m. \end{cases}$$

Note that the last recurrence in the system differs depending on whether n is odd or even.

40. In the context of Section 7.6, one can consider leaving probabilities as well as hitting probabilities. Let l_{ij} be the probability of exiting the transient states from transient state j when the chain starts in transient state i. If $x_i = \sum_{k=m+1}^{n} p_{ik}$ is the exit probability from state i and $X = \text{diag}(x)$ is the $m \times m$ diagonal matrix with x_i as its ith diagonal entry, then show that $L = (I - Q)^{-1} X$, where $L = (l_{ij})$. Calculate L in the illness-death model of Section 7.6.

41. An acceptance function $a : (0, \infty) \mapsto [0, 1]$ satisfies the functional identity $a(x) = xa(1/x)$. Prove that the detailed balance condition

$$\pi_i q_{ij} a_{ij} \quad = \quad \pi_j q_{ji} a_{ji}$$

holds if the acceptance probability a_{ij} is defined by

$$a_{ij} \quad = \quad a\left(\frac{\pi_j q_{ji}}{\pi_i q_{ij}}\right)$$

in terms of an acceptance function $a(x)$. Check that the Barker function $a(x) = x/(1 + x)$ qualifies as an acceptance function and that any acceptance function is dominated by the Metropolis acceptance function in the sense that $a(x) \leq \min\{x, 1\}$ for all x.

42. The Metropolis acceptance mechanism (7.19) ordinarily implies aperiodicity of the underlying Markov chain. Show that if the proposal distribution is symmetric and if some state i has a neighboring state j such that $\pi_i > \pi_j$, then the period of state i is 1, and the chain, if irreducible, is aperiodic. For a counterexample, assign probability $\pi_i = 1/4$ to each vertex i of a square. If the two vertices adjacent to a given vertex i are each proposed with probability 1/2, then show that all proposed steps are accepted by the Metropolis criterion and that the chain is periodic with period 2.

43. Consider the Cartesian product space $\{0, 1\} \times \{0, 1\}$ equipped with the probability distribution

$$(\pi_{00}, \pi_{01}, \pi_{10}, \pi_{11}) \quad = \quad \left(\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{8}\right).$$

Demonstrate that sequential Gibbs sampling does not satisfy detailed balance by showing that $\pi_{00} s_{00,11} \neq \pi_{11} s_{11,00}$, where $s_{00,11}$ and $s_{11,00}$ are entries of the matrix S for first resampling component one and then resampling component two.

44. In our analysis of convergence of the independence sampler, we asserted that the eigenvalues $\lambda_1, \ldots, \lambda_m$ satisfied the properties: (a) $\lambda_1 = 1 - 1/w_1$, (b) the λ_i are decreasing, and (c) $\lambda_m = 0$. Verify these properties.

45. Find the row and column eigenvectors of the transition probability matrix P for the independence sampler. Show that they are orthogonal in the appropriate inner products.

46. It is known that every planar graph can be colored by four colors [32]. Design, program, and test a simulated annealing algorithm to find a four coloring of any planar graph. (Suggestions: Represent the

graph by a list of nodes and a list of edges. Assign to each node a color represented by a number between 1 and 4. The cost of a coloring is the number of edges with incident nodes of the same color. In the proposal stage of the simulated annealing solution, randomly choose a node, randomly reassign its color, and recalculate the cost. If successful, simulated annealing will find a coloring with the minimum cost of 0.)

47. A Sudoku puzzle is a 9×9 matrix, with some entries containing predefined digits. The goal is to completely fill in the matrix, using the digits 1 through 9, in such a way that each row, column, and symmetrically placed 3×3 submatrix displays each digit exactly once. In mathematical language, a completed Sudoku matrix is a Latin square subject to further constraints on the 3×3 submatrices. The initial partially filled in matrix is assumed to have a unique completion. Design, program, and test a simulated annealing algorithm to solve a Sudoku puzzle.