Now define a Markov chain with states $0, 1, \ldots, n$ and transition probabilities

$$P_{0,0} = P_{n,n} = 1,$$

$$P_{ij} = \begin{cases} c_i & \text{if } j = i-1, \\ 1 - c_i & \text{if } j = i + k(i), \end{cases} \qquad i = 1, \ldots, n-1. \tag{4.6.6}$$

Let f_i denote the probability that this Markov chain ever enters state 0 given that it starts in state i. Then f_i satisfies

$$f_i = c_i f_{i-1} + (1 - c_i) f_{i+k(i)}, \qquad i = 1, \ldots, n-1,$$
$$f_0 = 1, \qquad f_n = 0.$$

Hence, as it can be shown that the above set of equations has a unique solution, it follows from (4.6.4) that if we take c_i equal to a_i for all i, then f_i will equal the Π_i of rule R, and from (4.6.5) if we let $c_i = b_i$, then f_i equals $\overline{\Pi}_i$. Now it is intuitively clear (and we defer a formal proof until Chapter 8) that the probability that the Markov chain defined by (4.6.6) will ever enter 0 is an increasing function of the vector $\underline{c} = (c_1, \ldots, c_{n-1})$. Hence, since $a_i \geq b_i$, $i = 1, \ldots, n$, we see that

$$\Pi_i \geq \overline{\Pi}_i \qquad \text{for all } i.$$

When $p \leq 1/n$, then $a_i \leq b_i$, $i = 1, \ldots, n-1$, and the above inequality is reversed.

THEOREM 4.6.4

Among the rules considered, the limiting expected position of the element requested is minimized by the transposition rule.

Proof Letting X denote the position of e_1, we have upon conditioning on whether or not e_1 is requested that the expected position of the requested element can be expressed as

$$E[\text{position}] = pE[X] + (1-p)\frac{E[1 + 2 + \cdots + n - X]}{n-1}$$
$$= \left(p - \frac{1-p}{n-1}\right)E[X] + \frac{(1-p)n(n+1)}{2(n-1)}.$$

Thus, if $p \geq 1/n$, the expected position is minimized by minimizing $E[X]$, and if $p \leq 1/n$, by maximizing $E[X]$. Since $E[X] = \sum_{i=0}^{n} P\{X > i\}$, the result follows from Proposition 4.6.3.

4.7 Time-Reversible Markov Chains

An irreducible positive recurrent Markov chain is stationary if the initial state is chosen according to the stationary probabilities. (In the case of an ergodic chain this is equivalent to imagining that the process begins at time $t = -\infty$.) We say that such a chain is in *steady state*.

Consider now a stationary Markov chain 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 $X_n, X_{n-1}, \ldots$. It turns out that this sequence of states is itself a Markov chain with transition probabilities P_{ij}^* defined by

$$P_{ij}^* = P\{X_m = j \mid X_{m+1} = i\}$$
$$= \frac{P\{X_{m+1} = i \mid X_m = j\} P\{X_m = j\}}{P\{X_{m+1} = i\}}$$
$$= \frac{\pi_j P_{ji}}{\pi_i}.$$

To prove that the reversed process is indeed a Markov chain we need to 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 the preceding is true, think of the present time as being time $m+1$. Then, since X_n, $n \geq 1$ is a Markov chain it follows that given the present state X_{m+1} the past state X_m and the future states $X_{m+2}, X_{m+3}, \ldots$ are independent. But this is exactly what the preceding equation states.

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

$$P_{ij}^* = \frac{\pi_j P_{ji}}{\pi_i}.$$

If $P_{ij}^* = P_{ij}$ for all i, j, then the Markov chain is said to be *time reversible*. The condition for time reversibility, namely, that

$$\pi_i P_{ij} = \pi_j P_{ji} \qquad \text{for all } i, j, \tag{4.7.1}$$

can be interpreted as stating 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 should be noted 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; that is, if $X_m = i$ and $X_{m-1} = j$, then a transition from i to j is observed if we are looking backward in time and one from j to i if we are looking forward in time.

If we can find nonnegative numbers, summing to 1, which satisfy (4.7.1), then it follows that the Markov chain is time reversible and the numbers represent the stationary probabilities. This is so since if

$$x_i P_{ij} = x_j P_{ji} \quad \text{for all } i, j \quad \sum_i x_i = 1, \tag{4.7.2}$$

then summing over i yields

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

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

EXAMPLE 4.7(A) ***An Ergodic Random Walk.*** We can argue, without any need for computations, that an ergodic chain with $P_{i,i+1} + P_{i,i-1} = 1$ 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 re-enter i from a higher state is by way of 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.

EXAMPLE 4.7(B) ***The Metropolis Algorithm.*** Let $a_j, j = 1, \ldots, m$ be positive numbers, and let $A = \sum_{j=1}^{m} a_j$. Suppose that m is large and that A is difficult to compute, and suppose we ideally want to simulate the values of a sequence of independent random variables whose probabilities are $p_j = a_j/A$, $j = 1, \ldots, m$. One way of simulating a sequence of random variables whose distributions converge to $\{p_j, j = 1, \ldots, m\}$ is to find a Markov chain that is both easy to simulate and whose limiting probabilities are the p_j. The *Metropolis algorithm* provides an approach for accomplishing this task.

Let $\boldsymbol{Q}$ be any irreducible transition probability matrix on the integers $1, \ldots, n$ such that $q_{ij} = q_{ji}$ for all i and j. Now define a Markov chain $\{X_n, n \geq 0\}$ as follows. If $X_n = i$, then generate a random variable that is equal to j with probability q_{ij}, $i, j = 1, \ldots, m$. If this random variable takes on the value j, then set X_{n+1} equal to j with probability $\min\{1, a_j/a_i\}$, and set it equal to i otherwise.

That is, the transition probabilities of $\{X_n, n \geq 0\}$ are

$$P_{ij} = \begin{cases} q_{ij} \min(1, a_j/a_i) & \text{if } j \neq i \\ q_{ii} + \sum_{j \neq i} q_{ij}\{1 - \min(1, a_j/a_i)\} & \text{if } j = i. \end{cases}$$

We will now show that the limiting probabilities of this Markov chain are precisely the p_j.

To prove that the p_j are the limiting probabilities, we will first show that the chain is time reversible with stationary probabilities $p_j, j = 1, \ldots, m$ by showing that

$$p_i P_{ij} = p_j P_{ji}.$$

To verify the preceding we must show that

$$p_i q_{ij} \min(1, a_j/a_i) = p_j q_{ji} \min(1, a_i/a_j).$$

Now, $q_{ij} = q_{ji}$ and $a_j/a_i = p_j/p_i$ and so we must verify that

$$p_i \min(1, p_j/p_i) = p_j \min(1, p_i/p_j).$$

However this is immediate since both sides of the equation are equal to $\min(p_i, p_j)$. That these stationary probabilities are also limiting probabilities follows from the fact that since $\boldsymbol{Q}$ is an irreducible transition probability matrix, $\{X_n\}$ will also be irreducible, and as (except in the trivial case where $p_i \equiv 1/n$) $P_{ii} > 0$ for some i, it is also aperiodic.

By choosing a transition probability matrix $\boldsymbol{Q}$ that is easy to simulate—that is, for each i it is easy to generate the value of a random variable that is equal to j with probability q_{ij}, $j = 1, \ldots, n$—we can use the preceding to generate a Markov chain whose limiting probabilities are a_j/A, $j = 1, \ldots, n$. This can also be accomplished without computing A.

Consider a graph having a positive number w_{ij} associated with each edge (i, j), and suppose that a particle moves from vertex to vertex in the following manner: If the particle is presently at vertex i then it will next move to vertex j with probability

$$P_{ij} = w_{ij} \Big/ \sum_j w_{ij}$$

where w_{ij} is 0 if (i, j) is not an edge of the graph. The Markov chain describing the sequence of vertices visited by the particle is called a random walk on an edge weighted graph.

PROPOSITION 4.7.1

Consider a random walk on an edge weighted graph with a finite number of vertices. If this Markov chain is irreducible then it is, in steady state, time reversible with stationary probabilities given by

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

Proof The time reversibility equations

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

reduce to

$$\frac{\pi_i w_{ij}}{\sum_k w_{ik}} = \frac{\pi_j w_{ji}}{\sum_k w_{jk}}$$

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

$$\frac{\pi_i}{\sum_k w_{ik}} = \frac{\pi_j}{\sum_k w_{jk}}$$

implying that

$$\pi_i = c \sum_k w_{ik}$$

which, since $\sum \pi_i = 1$, proves the result.

Example 4.7(c) Consider a star graph consisting of r rays, with each ray consisting of n vertices. (See Example 1.9(C) for the definition of a star graph.) Let leaf i denote the leaf on ray i. Assume that a particle moves along the vertices of the graph in the following manner. Whenever it is at the central vertex 0, it is then equally likely to move to any of its neighbors. Whenever it is on an internal (nonleaf) vertex of a ray, then it moves towards the leaf of that ray with probability p and towards 0 with probability $1 - p$. Whenever it is at a leaf, it moves to its neighbor vertex with probability 1. Starting at vertex 0, we are interested in finding the expected number of transitions that it takes to visit all the vertices and then return to 0.

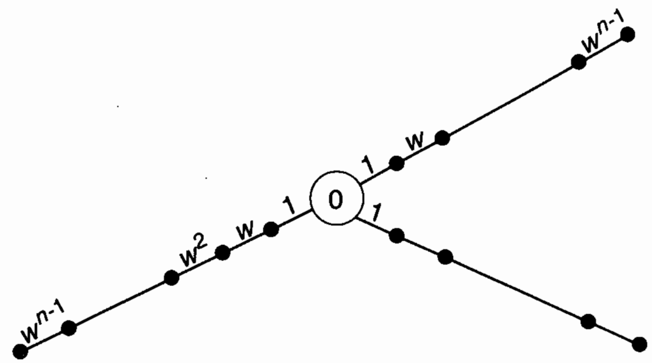

Figure 4.7.1. A star graph with weights: $w = p/(1 - p)$.

To begin, let us determine the expected number of transitions between returns to the central vertex 0. To evaluate this quantity, note the Markov chain of successive vertices visited is of the type considered in Proposition 4.7.1. To see this, attach a weight equal to 1 with each edge connected to 0, and a weight equal to w^i on an edge connecting the ith and $(i + 1)$st vertex (from 0) of a ray, where $w = p/(1 - p)$ (see Figure 4.7.1). Then, with these edge weights, the probability that a particle at a vertex i steps from 0 moves towards its leaf is $w^i/(w^i + w^{i-1}) = p$.

Since the total of the sum of the weights on the edges out of each of the vertices is

$$r + r\left[\sum_{i=1}^{n-1} (w^{i-1} + w^i) + w^{n-1}\right] = \frac{2r(1 - w^n)}{1 - w},$$

and the sum of the weights on the edges out of vertex 0 is r, we see from Proposition 4.7.1 that

$$\pi_0 = \frac{1 - w}{2(1 - w^n)}.$$

Therefore, μ_{00}, the expected number of steps between returns to vertex 0, is

$$\mu_{00} = 1/\pi_0 = \frac{2(1 - w^n)}{1 - w}.$$

Now, say that a new cycle begins whenever the particle returns to vertex 0, and let X_j be the number of transitions in the jth cycle, $j \geq 1$. Also, fix i and let N denote the number of cycles that it takes for the particle to visit leaf i and then return to 0. With these definitions, $\sum_{j=1}^{N} X_j$ is equal to the number of steps it takes to visit leaf i and then return to 0. As N is clearly a stopping time for the X_j, we obtain from Wald's equation that

$$E\left[\sum_{j=1}^{N} X_j\right] = \mu_{00} E[N] = \frac{2(1-w^n)}{1-w} E[N].$$

To determine $E[N]$, the expected number of cycles needed to reach leaf i, note that each cycle will independently reach leaf i with probability $\frac{1-1/w}{r[1-(1/w)^n]}$ where $1/r$ is the probability that the transition from 0 is onto ray i, and $\frac{1-1/w}{1-(1/w)^n}$ is the (gambler's ruin) probability that a particle on the first vertex of ray i will reach the leaf of that ray (that is, increase by $n-1$) before returning to 0. Therefore N, the number of cycles needed to reach leaf i, is a geometric random variable with mean $r[1-(1/w)^n]/(1-1/w)$, and so

$$E\left[\sum_{j=1}^{N} X_j\right] = \frac{2r(1-w^n)[1-(1/w)^n]}{(1-w)(1-1/w)} = \frac{2r[2-w^n-(1/w)^n]}{2-w-1/w}.$$

Now, let T denote the number of transitions that it takes to visit all the vertices of the graph and then return to vertex 0. To determine $E[T]$ we will use the representation

$$T = T_1 + T_2 + \cdots + T_r,$$

where T_1 is the time to visit the leaf 1 and then return to 0; T_2 is the additional time from T_1 until both the leafs 1 and 2 have been visited and the process returned to vertex 0; and, in general, T_i is the additional time from T_{i-1} until all of the leafs $1, \ldots, i$ have been visited and the process returned to 0. Note that if leaf i is not the last of the leafs $1, \ldots, i$ to be visited, then T_i will equal 0, and if it is the last of these leafs to be visited, then T_i will have the same distribution as the time until a specified leaf is first visited and the process then returned to 0. Hence, upon conditioning on whether leaf i is the last of leafs $1, \ldots, i$ to be visited (and the probability of this event is clearly $1/i$), we obtain from the preceding that

$$E[T] = \frac{2r[2-w^n-1/w^n]}{2-w-1/w} \sum_{i=1}^{r} 1/i.$$

If we try to solve Equations (4.7.2) for an arbitrary Markov chain, it will usually turn out that no solution exists. For example, from (4.7.2)

$$x_i P_{ij} = x_j P_{ji},$$
$$x_k P_{kj} = x_j P_{jk},$$

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

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

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

$$P_{ik}P_{kj}P_{ji} = P_{ij}P_{jk}P_{ki} \qquad \text{for all } i, j, k, \tag{4.7.3}$$

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 occur 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 (4.7.3).

In fact we can show the following.

THEOREM 4.7.2

A stationary Markov chain is time reversible if, and only if, starting in state i, any path back to i has the same probability as the reversed path, for all i. That is, if

$$P_{i,i_1}P_{i_1,i_2}\cdots P_{i_k,i} = P_{i,i_k}P_{i_k,i_{k-1}}\cdots P_{i_1,i} \tag{4.7.4}$$

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

Proof The proof of necessity is as indicated. To prove sufficiency fix states i and j and rewrite (4.7.4) 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 $i_1, i_2, \ldots, i_k$ yields

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