Construction of Transition Matrices of Reversible Markov Chains

by

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A Major Paper

Submitted to the Faculty of Graduate Studies

through the Department of Mathematics and Statistics

in Partial Fulfillment of the Requirements for

the Degree of Master of Science at the

University of Windsor

Windsor, Ontario, Canada

2009

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Abstract

This major paper reviews methods for generating transition matrices of reversible Markov processes, and introduces several new methods. A method to check for reversibility from a given finite state transition matrix is presented through the use of a computer program in R.

Acknowledgments

I would like to express my most profound gratitude to my supervisor, Dr. Hlynka, whose selfless help, stimulating suggestions and encouragement helped me in all the time of research for and writing of this major paper. I appreciate him for awarding me the research funding for this research and for understanding me when I am at the important point in my life.

Moreover, thanks to Dr. Nkurunziza, as the department reader.

Especially thanks to my unborn baby. Your existence imparts valuable life to me and the whole family.

My last thanks is to my beloved husband Eric for your endless love.

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Chapter 1

Introduction

1.1 Reversible Markov Chains

According to Ross, a stochastic process $\{X_n, n = 0, 1, 2, \ldots\}$ such that

$$P\{X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \ldots, X_1 = i_1, X_0 = i_0\} = P\{X_{n+1} = j | X_n = i\}$$

is a Markov chain.

Some books that discuss reversibility include Aldous and Fill (2002), Kelly (1979), Nelson (1995), Kao (1997), and Wolff (1989). Other books will be mentioned as they are referred to in this major paper.

According to Strook (2005), a class of Markov processes is said to be reversible if, on every time interval, the distribution of the process is the same when it is run backward as when it is run forward. That is, for any $n \geq 0$ and $(i_0, \cdots, i_n) \in S^{(n+1)}$, in the discrete time setting,

$$P(X_m = i_m \text{ for } 0 \leq m \leq n) = P(X_{(n-m)} = i_m \text{ for } 0 \leq m \leq n) \tag{1.1}$$

and in the continuous time setting,

$$P(X(t_m) = i_m \text{ for } 0 \leq m \leq n) = P(X(t_n - t_m) = i_m \text{ for } 0 \leq m \leq n) \tag{1.2}$$

whenever $0 = t_0 \leq \cdots \leq t_n$. Indeed, depending on whether the setting is that of discrete or continuous time, we have

$$P(X_0 = i, X_n = j) = P(X_0 = j, X_n = i)$$

or

$$P(X(0) = i, X(t) = j) = P(X(t) = i, X(0) = j)$$

In fact, reversibility says that, depending on the setting, the joint distribution of (X_0, X_n) (or $(X(0), X(t))$) is the same as that of (X_n, X_0) (or $(X(t), X(0))$).

If P is the transition probability matrix, then , by taking $n = 1$ in equation (1.1), we see that

$$\pi_i p_{ij} = P(X_0 = i \cap X_1 = j) = P(X_0 = j \cap X_1 = i) = \pi_j p_{ji}.$$

That is, P satisfies

$$\pi_i p_{ij} = \pi_j p_{ji}, \text{ the condition of } \textbf{detailed balance}. \tag{1.3}$$

Conversely, (1.3) implies reversibility. To see this, one works by induction on $n \geq 1$ to check that

$$\pi_{i_0} p_{i_0 i_1} \cdots p_{i_{n-1} i_n} = \pi_{i_n} p_{i_n i_{n-1}} \cdots p_{i_1 i_0},$$

which is equivalent to (1.1). Further, we can verify that a reversible process is stationary since it has the invariant distributions.

We summarize the above discussion in the form of a theorem.

The following statement is from Rubinstein and Kroese (2007).

Theorem 1.1.1.

A stationary process is reversible if and only if there exists a positive collection of numbers $\{\pi_i\}$ *summing to unity such that*

$$\pi_i p_{ij} = \pi_j p_{ji} \textit{ for all } i, j \in S$$

Whenever such a collection exists, it is the equilibrium distribution.

According to Rubinstein (2007): "Intuitively, $\pi_i p_{ij}$ can be thought of as the probability flux from state i to state j. Thus the detailed balance equations say that the probability flux from state i to state j equals that from state j to state i." This interpretation is helpful for constructing transition matrices of reversible Markov chains.

1.2 Technology to check reversibility

The detailed balance equation allows us to determine if a process is reversible based on the transition probability matrix and the limiting probabilities. We designed a method to check the reversibility of a Markov chain based on the detailed balance equations. Specifically, we use an R program (R 2.9.0) to help compute the limiting probabilities and related calculations.

Henceforth, when we mention *reversible matrix* or *a matrix which is reversible*, we actually mean *the transition matrix of a reversible Markov process*. This terminology is used for conciseness.

1.2.1 Calculation of limiting probabilities

Let P be the transition matrix of a Markov chain. Let $P^{(n)}$ be the n step transition matrix. Let P^n be the n-th power of the transition matrix. Let $\Pi = \lim_{n\to\infty} P^n$, if the limit exists. Let $\underline{\pi}$ be the limiting probability vector, if it exists.
Then we know that

$$\Pi = \lim_{n\to\infty} P^{(n)} = \lim_{n\to\infty} P^n$$

and each common row of Π, is $\underline{\pi}$, the limiting vector.

Property 1.2.1. *A Markov chain with transition matrix P is reversible if $\Pi * P$ is symmetric where $*$ means component-wise multiplication.*

Proof. Let $R = \Pi^T * P$.

$$\Pi = \begin{bmatrix} \pi_1 & \pi_2 & \pi_3 & \cdots \\ \pi_1 & \pi_2 & \pi_3 & \cdots \\ \pi_1 & \pi_2 & \pi_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Then

$$\begin{aligned} R = \Pi^T * P &= \begin{bmatrix} \pi_1 & \pi_2 & \pi_3 & \cdots \\ \pi_1 & \pi_2 & \pi_3 & \cdots \\ \pi_1 & \pi_2 & \pi_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} * \begin{bmatrix} p_{11} & p_{12} & p_{13} & \cdots \\ p_{21} & p_{22} & p_{23} & \cdots \\ p_{31} & p_{32} & p_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \\ &= \begin{bmatrix} \pi_1 p_{11} & \pi_1 p_{12} & \pi_1 p_{13} & \cdots \\ \pi_2 p_{21} & \pi_2 p_{22} & \pi_2 p_{23} & \cdots \\ \pi_3 p_{31} & \pi_3 p_{32} & \pi_3 p_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \end{aligned}$$

If we get a symmetric matrix, that is, if $\pi_i p_{ij} = \pi_j p_{ji}$ for all i, j, then the detailed balance equations are satisfied. Thus the transition matrix P is reversible. Otherwise, P is not reversible. □

Technically, with the aid of software, for an irreducible Markov chain, if we compute P^n to a large enough number of power n, say 100, then usually we will get a matrix which has common rows, and each row is the limiting vector $\underline{\pi}$. If the rows are not all equal, we may need to take n larger to see if we get the desired matrix. If not, it is possible that we improperly entered the transition matrix since, according to Allen (2003), a finite Markov process always has stationary distribution.

1.2.2 Checking for reversibility

Consider as an example the transition matrix $P = \begin{bmatrix} .5 & .25 & .25 \\ .5 & 0 & .5 \\ .25 & .25 & .5 \end{bmatrix}$.

In R, we apply the commands as in Figure 1.1

```
> power=function(A,n){Ans=diag(dim(A)[1]); for (i in 1:n){Ans=Ans%*%A};Ans}
> P=matrix(c(.5,.5,.25,.25,0,.25,.25,.5,.5),3,3)
> P
     [,1] [,2] [,3]
[1,] 0.50 0.25 0.25
[2,] 0.50 0.00 0.50
[3,] 0.25 0.25 0.50
> P100=power(P,100)
> P100
     [,1] [,2] [,3]
[1,]  0.4  0.2  0.4
[2,]  0.4  0.2  0.4
[3,]  0.4  0.2  0.4
```

Figure 1.1: Computing limiting probabilities with R

As we see, the limiting vector of P is $\underline{\pi} = (0.4, 0.2, 0.4)$. We transpose P^{100} and compute $(P^{100})^T * P$.

In R, we compute this procedure as in Figure 1.2 (continued from Figure 1.1)

```
> t(P100)*P
     [,1] [,2] [,3]
[1,]  0.2  0.1  0.1
[2,]  0.1  0.0  0.1
[3,]  0.1  0.1  0.2
```

Figure 1.2: Checking symmetry with R

In this example, we get a symmetric matrix, and conclude that P is reversible.

So far, we have given a method to check the reversibility of a transition matrix with aid of an R program. In the later discussion of ways to construct reversible matrices, we will always use this method to test the validity of the examples.

For the remainder of this paper, we will assume that our Markov chains are all irreducible, aperiodic, and positive recurrent. Thus the limiting vector will always exist, be nonzero, and not depend on the initial state.

Although we will be dealing mainly with reversibility in discrete time Markov chains and probability transition matrices, most of the results hold for continuous time Markov processes and rate matrices (infinitesimal generators).

Chapter 2

Kolmogorov's Criterion and Symmetric Zeros

2.1 Kolmogorov's Criterion

Kolmogorov's Criterion is a method to check and the reversibility of a transition matrix, without requiring knowledge of the limiting probability vector. It can also be used as a method to construct transition matrices of reversible Markov process and to validate some of the other methods in this paper.

The following is taken from Ross (2002). It is included here since the result is used frequently in this paper.

Theorem 2.1.1. *(Kolmogorov Criterion) A stationary Markov chain is reversible if and only if, any path starting from state i and back to i has the same probability as the path going in the reverse direction. That is, the chain is reversible iff*

$$p_{ii_1}p_{i_1i_2}\cdots p_{i_ki} = p_{ii_k}p_{i_ki_{k-1}}\cdots p_{i_1i} \tag{2.1}$$

$\forall k$ *and* $i, i_1, i_2, \cdots, i_k \in S$.

Proof. We prove the necessity first.

If a Markov chain is reversible, the detailed balance equations are

$$\pi_i p_{ii_1} = \pi_{i_1} p_{i_1 i}$$

$$\pi_{i_1} p_{i_1 i_2} = \pi_{i_2} p_{i_2 i_1}$$

$$\vdots$$

$$\pi_{i_{k-1}} p_{i_{k-1} i_k} = \pi_{i_k} p_{i_k i_{k-1}}$$

$$\pi_{i_k} p_{i_k i} = \pi_i p_{ii_k}$$

$\forall k$ and $i, i_1, i_2, \cdots, i_k \in S$.

Multiply both sides of the reversibility equations together, and cancel out the common part $\pi_i \pi_{i_1} \cdots \pi_{i_k}$ to get

$$p_{ii_1} p_{i_1 i_2} \cdots p_{i_k i} = p_{ii_k} p_{i_k i_{k-1}} \cdots p_{i_1 i}.$$

$\forall k$ and $i, i_1, i_2, \cdots, i_k \in S$.

Next we prove sufficiency.

Fix states i and j and rewrite Equation (2.1) as

$$p_{ii_1} p_{i_1 i_2} \cdots p_{i_k j} p_{ji} = p_{ij} p_{ji_k} p_{i_k i_{k-1}} \cdots p_{i_1 i} \tag{2.2}$$

Now $p_{ii_1} p_{i_1 i_2} \cdots p_{i_k j}$ is the probability of starting from state i, moving to state j after k steps and then going into state i at $(k+1)th$ step. Similarly $p_{ji_k} p_{i_k i_{k-1}} \cdots p_{i_1 i}$ is the probability of starting from state j, moving to state i after k steps and then moving into state j at $(k+1)th$ step. Hence, summing both sides of Equation (2.2) over all intermediate states $i_1, i_2, \cdots, i_k$ yields

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

Summing over k shows that

$$p_{ji}\frac{\sum_{k=1}^{n} p_{ij}^{k}}{n} = p_{ij}\frac{\sum_{k=1}^{n} p_{ji}^{k}}{n}$$

Letting $n \to \infty$ yields

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

thus showing that the chain is reversible. □

Knowing this powerful condition, we can construct transition matrices of Markov chain by making the probability of one path equal to the probability of its reversed path. However, Kolmogorov's condition is mainly used for reversibility verification and proof.

Example 2.1.1.

I simply give a 3×3 *transition matrix for example.*

$$P = \begin{bmatrix} .2 & .4 & .4 \\ .3 & .4 & .3 \\ .5 & .5 & 0 \end{bmatrix}$$

Thus $p_{12}p_{23}p_{31} = (.4)(.3)(.5) = p_{13}p_{32}p_{21} = (.4)(.5)(.3)$

For a 3×3 *transition matrix, it turns out that only one detailed balance equation has to be checked. So* P *is reversible.*

2.2 Number of checks required.

We believe that the following result is new.

Property 2.2.1. *For an* $n \times n$ *transition matrix, the number of distinct Kolmogorov equations that must be checked is*

$$\sum_{i=3}^{n} \binom{n}{i} \frac{(i-1)!}{2}.$$

Proof. We note that using Kolmogorov's condition to check a 2×2 transition matrix means checking that $p_{12}p_{21} = p_{21}p_{12}$. For a two-state matrix, we even do not need to check at all because the probabilities always satisfy Kolmogorov's condition, i.e., a two-state transition matrix is always reversible. Then we are led to ask that how many equations need to be checked for larger state space matrices.

We note that using Kolmogorov's condition to check a 3×3 matrix is very simple because the number of equations to be checked is only one. One finds that all the different paths of Kolmogorov's condition reduce to a single equation.

For a 4×4 transition matrix, we must check all three state paths and all four state paths. As to the three state paths, we choose any three states out of four and for each three-state path, we check only once, while for the four-state paths, we can assume that starting state is fixed. Then there are 3! paths for the other states. However, since the other side of equation is just the reversed path, we are reduced to $\frac{3!}{2}$ paths involving four states. In total, we need to check $\left(\binom{4}{3} + \frac{3!}{2} = 7\right)$ equations.

Similarly for a 5×5 transition matrix, we must check all the three-state paths, four-state paths and five-state paths, that is $\left(\binom{5}{3} + \binom{5}{4}\frac{(4-1)!}{2} + \frac{(5-1)!}{2}\right) = 37$ equations to ensure the validity of Kolmogorov's condition.

The same argument works for any $n \times n$ transition matrix. □

The following Table 2.1 shows this relation clearly.

This gives an interesting sequence as shown in the right column of the table.

The sequence was checked at The On-Line Encyclopedia of Integer Sequences, a web site on integer sequences. For anyone who is interested, please see

http://www.research.att.com/~njas/sequences/Seis.html

The sequence already existed there but had only one explanation. A second explanation was therefore added to note that it gives the number of Kolmogorov type

$Number of states$	$Number of checking$
0	0
1	0
2	0
3	1
4	7
5	37
6	197
7	1172
8	8018
9	62814
10	556014

Table 2.1: Sequence of checking

equations that must be checked for reversibility. The note appears on the web site as follows.

A002807 Sum_{k=3..n} (k-1)!*C(n,k)/2.

(Formerly M4420 N1867)

0, 0, 0, 1, 7, 37, 197, 1172, 8018, 62814, 556014, 5488059, 59740609, 710771275, 9174170011, 127661752406, 1904975488436, 30341995265036, 513771331467372, 9215499383109573, 174548332364311563, 3481204991988351553, 72920994844093191553, 160059637159039967178

COMMENT Maximal number of cycles in complete graph on n nodes.

- Erich Friedman (erich.friedman(AT)stetson.edu).

Number of equations that must be checked to verify reversibility of

an n state Markov chain using the Kolmogorov criterion

- From Qian Jiang (jiang1h(AT)uwindsor.ca), Jun 08 2009

2.3 Nonsymmetric zero entries

Another useful result is the following.

Theorem 2.3.1.

A transition matrix is not reversible if there exists any nonsymmetric zero entry in the matrix.

Proof.

The proof is quite simple because either the detailed balance equation or the Kolmogorov's condition is violated in such cases. □

Example 2.3.1.

Consider the transition matrix

$$P = \begin{bmatrix} .5 & .3 & .1 & .1 \\ .4 & .2 & .1 & .3 \\ .1 & 0 & .7 & .2 \\ .2 & .1 & .3 & .4 \end{bmatrix}$$

We do not need to bother the checking method in Chapter 1 and we are sure that P is not reversible since there is a 0 *entry in the (3,2) position which has a non-zero in the (2,3) position.*

Chapter 3

Metropolis-Hastings Algorithm

3.1 Discussion and Algorithm

According to Rubinstein (2007) "The main idea behind the Metropolis-Hastings algorithm is to simulate a Markov chain such that the stationary distribution of this chain coincides with the target distribution."

Such a problem arises naturally: Given a probability distribution $\{\pi_i\}$ on a state space S, how can we construct a Markov chain on S that has $\{\pi_i\}$ as a stationary distribution, and prove that such a Markov chain is reversible with respect to $\{\pi_i\}$?

According to Evans and Rosenthal (2004), given $X_n = i$, the Metropolis-Hastings algorithm computes the value X_{n+1} as follows.

- We are given $\underline{\pi}$. Pick any Markov chain $[q_{ij}]$ transition matrix with size given by the number of states.
- Choose $Y_{n+1} = j$ according to the Markov chain $\{q_{ij}\}$.
- Set $\alpha_{ij} = \min\left\{1, \frac{\pi_j q_{ji}}{\pi_i q_{ij}}\right\}$ (the acceptance probability)

- With probability α_{ij}, let $X_{n+1} = Y_{n+1} = j$ (i.e.,accepting the proposal Y_{n+1}). Otherwise, with probability $1 - \alpha_{ij}$, let $X_{n+1} = X_n = i$ (i.e. rejecting the proposal Y_{n+1}).

3.2 Main Property

Property 3.2.1. *The Metropolis-Hastings algorithm results in a Markov chain $X_0, X_1, X_2, \cdots$, which has $\{\pi_i\}$ as a stationary distribution, and the resulting Markov chain is* reversible *with respect to $\{\pi_i\}$, i.e.,*

$$\pi_i P(X_{n+1} = j|X_n = i) = \pi_j P(X_{n+1} = i|X_n = j),$$

for $i, j \in S$.

Proof. (Evans and Rosenthal)
We will prove the reversibility of the Markov chain first, and then show that such $\{\pi_i\}$ is the stationary distribution for the chain.

$\pi_i P(X_{n+1} = j|X_n = i) = \pi_j P(X_{n+1} = i|X_n = j)$, is naturally true if $i = j$, so we will assume that $i \neq j$.

But if $i \neq j$, and $X_n = i$, then the only way we can have $X_{n+1} = j$ is if $Y_{n+1} = j$(i.e., we propose the state j, which we will do with probability p_{ij}).Also we accept this proposal (which we will do with probability α_{ij}. Hence

$$P(X_{n+1} = j|X_n = i) = q_{ij}\alpha_{ij} = q_{ij}\min\left\{1, \frac{\pi_j q_{ji}}{\pi_i q_{ij}}\right\} = \min\left\{q_{ij}, \frac{\pi_j q_{ji}}{\pi_i}\right\}.$$

It follows that $\pi_i P(X_{n+1} = j|X_n = i) = \min\{\pi_i q_{ij}, \pi_j q_{ji}\}$.

Similarly, we compute that $\pi_j P(X_{n+1} = i|X_n = j) = \min\{\pi_j q_{ji}, \pi_i q_{ij}\}$.

It follows that $\pi_i P(X_{n+1} = j|X_n = i) = \pi_j P(X_{n+1} = i|X_n = j)$ is true for all $i, j \in S$, i.e., the Markov chain made from the Metropolis-Hastings algorithm is a reversible chain with respect to $\{\pi_i\}$.

Now we shall prove that if a Markov chain is reversible with respect to $\{\pi_i\}$, then $\{\pi_i\}$ is a stationary distribution for the chain.

We compute, using reversibility, that for any $j \in S$,

$$\sum_{i\in S} \pi_i p_{ij} = \sum_{i\in S} \pi_j p_{ji} = \pi_j \sum_{i\in S} p_{ji} = \pi_j(1) = \pi_j.$$

Hence, $\{\pi_i\}$ is a stationary distribution. □

Example 3.2.1. *We have not found any book which give matrix type examples. We present one such example here.*

Step 1. Given an arbitrary $\underline{\pi}$

$$\underline{\pi} = (.1, .2, .3, .4)$$

Step 2. Make up a Markov chain $\{Y_i\}$ *which has transition matrix* Q *(a simple one).*

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

Step 3. Calculate α_{ij}*, leaving the diagonal empty.*

$$\alpha_{12} = min\left\{1, \frac{\pi_2 q_{21}}{\pi_1 q_{12}}\right\} = min\left\{1, \frac{.2(.2)}{.1(.2)}\right\} = 1$$

Similarly, we compute out all the $\{\alpha_{ij}\}$ *and get matrix* $\underline{\alpha}$

$$\underline{\alpha} = \begin{bmatrix} \_ & 1 & 1 & 1 \\ \frac{1}{2} & \_ & \frac{1}{2} & 1 \\ 1 & 1 & \_ & \frac{4}{9} \\ \frac{3}{16} & \frac{3}{4} & 1 & \_ \end{bmatrix}$$

Step 4. Multiply Q and $\underline{\alpha}$ (here we use the element by element multiplication, not the matrix product). Then fill in the diagonals so the rows sum to one and get a new transition matrix P.

$$P = \begin{bmatrix} .2 & .2 & .3 & .3 \\ .1 & .45 & .15 & .3 \\ .1 & .1 & \frac{2}{3} & \frac{2}{15} \\ \frac{3}{40} & \frac{3}{20} & .1 & \frac{27}{40} \end{bmatrix}$$

Now we are to check the reversible nature of P using R as in Section 1.2.2.

$$P^{100} = \begin{bmatrix} 0.1 & 0.2 & 0.3 & 0.4 \\ 0.1 & 0.2 & 0.3 & 0.4 \\ 0.1 & 0.2 & 0.3 & 0.4 \\ 0.1 & 0.2 & 0.3 & 0.4 \end{bmatrix},$$

which means the limiting vector is $\underline{\pi} = [0.1, 0.2, 0.3, 0.4]$. It is identical to the limiting vector we start with.

Also

$$(P^{100})^T * P = \begin{bmatrix} 0.02 & 0.02 & 0.03 & 0.03 \\ 0.02 & 0.09 & 0.03 & 0.06 \\ 0.03 & 0.03 & 0.20 & 0.04 \\ 0.03 & 0.06 & 0.04 & 0.27 \end{bmatrix},$$

is a symmetric matrix and that verifies the reversibility of P.

Chapter 4

Simple Reversible Matrices

4.1 Symmetric transition matrices

The following result is well known. See Kijima (1997), for example.

Property 4.1.1. *Markov chains defined by symmetric transition matrices are always reversible, i.e.,*

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

is always true for all $i, j \in S$.

Proof.

Suppose that a transition matrix itself is symmetric, i.e. $p_{ij} = p_{ji}$ for all i and j. Then, since $\sum_j p_{ij} = \sum_j p_{ji} = 1$, the transition matrix is doubly stochastic, i.e. a square matrix of nonnegative real numbers, each of whose rows and columns sums to 1. The stationary distribution of a finite, doubly stochastic matrix is uniform (omit proof here). Specifically, $\pi_i = \frac{1}{n}$, where n is the number of states.

Hence, $p_{ij}\pi_i = p_{ji}\pi_j$ holds for all $i, j \in S$, the corresponding Markov chain is reversible.

□

Example 4.1.1. *Given a* $4 * 4$ *symmetric transition matrix* P

$$P = \begin{bmatrix} .3 & .2 & .1 & .4 \\ .2 & .5 & 0 & .3 \\ .1 & 0 & .7 & .2 \\ .4 & .3 & .2 & .1 \end{bmatrix}$$

The uniform stationary distribution $\pi_1 = \pi_2 = \pi_3 = \pi_4 = .25$*, thus the reversibility follows.*

4.2 Equal row entries (except diagonal)

We believe the following result is new (as we have not found it in the literature).

Property 4.2.1. *A transition matrix which has equal entries within each row, except perhaps the diagonal entry, is reversible.*

Proof. Consider a transition matrix with states $\{S\}$, with equal row entries, except perhaps the diagonal ones. A path from state i back to state i has probability

$$p_{ij}p_{jk} \cdots p_{lm}p_{mi} \tag{4.1}$$

$\forall i, j, \cdots, l, m \in S$.

Here we are always supposed to transit from one state to different state in one step, i.e., we are not stuck at any state (so the diagonal entries need not equal the other row entries), which is consistent with Kolmogorov's condition.

If we reverse this path, it will be

$$p_{im}p_{ml} \cdots p_{kj}p_{ji} \tag{4.2}$$

$\forall i, j, \cdots, l, m \in S$

Since the row entries are equal, we can match every entry in (4.1) with an entry in (4.2), by simply finding the same row subscript.

Therefore (4.1)=(4.2) for any number of steps of the path, which clearly satisfies Kolmogorov's criterion. We conclude that a Markov transition matrix with equal row entries (except possibly the diagonal entries) is reversible. □

Example 4.2.1. *We make up a transition matrix P which has equal row entries,*

$$P = \begin{bmatrix} .5 & .25 & .25 \\ .3 & .4 & .3 \\ .125 & .125 & .75 \end{bmatrix}$$

We check its reversibility using R and get the limiting vector is

$$\underline{\pi} = (0.2608696, 0.2173913, 0.5217391)$$

and

$$(P^{100})^T * P = \begin{bmatrix} 0.13043478 & 0.06521739 & 0.06521739 \\ 0.06521739 & 0.08695652 & 0.06521739 \\ 0.06521739 & 0.06521739 & 0.39130435 \end{bmatrix}.$$

P is verified to be reversible.

4.3 Equal column entries (except diagonal)

We believe the following result is new.

Property 4.3.1. *A transition matrix which has equal entries within each column, except possibly the diagonal entry, is reversible.*

Proof. The proof is similar to the proof for rows. □

Example 4.3.1.

$$P = \begin{bmatrix} .3 & .4 & .3 \\ .25 & .45 & .3 \\ .25 & .4 & .35 \end{bmatrix}.$$

We can conclude its reversibility since the entries within each column (except the diagonal) are all equal.

Another interesting example in this category worth mentioning is

$$P = \begin{bmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{8} & \cdots \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{8} & \cdots \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{8} & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix},$$

which has equal entries in each column, identical rows and each row is an infinite sequence. Such a matrix obviously has as its limiting vector any row of the matrix so if we wish to find a matrix with a given $\underline{\pi}$, we can construct such a matrix by taking the rows all equal to $\underline{\pi}$. This is the only infinite state transition matrix which appears in this paper. This matrix is reversible since all the columns have equal entries. We can then modify this matrix, using our methods, to create many other reversible transition matrices.

4.4 Reversible Birth-Death and Quasi-Birth-Death Process(QBD)

According to Kelly (1979), any birth-death process is reversible iff the detailed balance equation is satisfied. We omit the proof here. For the general proof, see Kelly(1979).

Thus, consider a birth-death process which has common birth probability λ and common death probability μ, and the transition matrix

$$P = \begin{bmatrix} -\lambda & \lambda & 0 & 0 & \cdots \\ \mu & -(\mu+\lambda) & \lambda & 0 & \cdots \\ 0 & \mu & -(\mu+\lambda) & \lambda & \cdots \\ 0 & 0 & \mu & -(\mu+\lambda) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \tag{4.3}$$

The local balance equation $\pi_i(\lambda_i + \mu_i) = \pi_{i+1}\mu_{i+1} + \pi_{i-1}\mu_{i-1}$ is always satisfied thus the Markov process is reversible.

Then we consider a simple quasi birth-death process with two levels of states which defined by transition matrix

$$Q = \begin{bmatrix} * & \lambda & a & 0 & 0 & \cdots \\ \mu & * & \lambda & a & 0 & \cdots \\ b & \mu & * & \lambda & a & \cdots \\ 0 & b & \mu & * & \lambda & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \tag{4.4}$$

where we use (*) in the place of diagonal entries to make the matrix look clear.

This is a quasi birth-death process of the form

$$Q = \begin{bmatrix} A_1 & A_0 & 0 & 0 & \dots \\ A_2 & A_1 & A_0 & 0 & \dots \\ 0 & A_2 & A_1 & A_0 & \dots \\ 0 & 0 & A_2 & A_1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \tag{4.5}$$

where $A_0 = \begin{bmatrix} a & 0 \\ \lambda & a \end{bmatrix}$, $A_1 = \begin{bmatrix} * & \lambda \\ \mu & * \end{bmatrix}$, $A_2 = \begin{bmatrix} b & \mu \\ 0 & b \end{bmatrix}$.

This model would be appropriate for a queueing system which allows arrivals of single or paired customers and allows service of single or paired customers.

Usually, to find the solution of stationary distribution of QBD process is not very easy. See Nelson (1995, Chapter 9) and Jain (2006, Chapter 8). However, if the QBD is reversible, then to work out the stationary distribution π_i would be quite simple by using the detailed balance equation and the fact that $\sum_i \pi_i = 1$.

Here we are interested in finding a and b such that Q is reversible. Again from the detailed balance equations, if Q is reversible, then

$$\frac{\pi_{i+1}}{\pi_i} = \frac{p_{i,i+1}}{p_{i+1,i}} = \frac{\lambda}{\mu},$$

that is, Q has the same stationary distribution as that of P. Also we get

$$\frac{a}{b} = \frac{p_{i,i+2}}{p_{i+2,i}} = \frac{\pi_{i+2}}{\pi_i} = \frac{\pi_{i+2}}{\pi_{i+1}}\frac{\pi_{i+1}}{\pi_i} = (\frac{\lambda}{\mu})^2.$$

In summary, we state the above discussion as a property, which we believe to be new.

Property 4.4.1. *For a Quasi-Birth-Death process which is defined by transition matrix Q, where Q has λ, μ as the first level transition probabilities and a, b as the second ones (just as shown in equation 4.4), if $\frac{a}{b} = (\frac{\lambda}{\mu})^2$, then Q is the transition matrix of a reversible Quasi-Birth-Death process.*

This result can be valuable to check the validity and accuracy of iterative methods for solving QBD's.

Chapter 5

Scaling of Transition Rates

5.1 Scale symmetric pairs

According to Nelson (1995), we introduce the following method.

Property 5.1.1. *By changing the symmetric pairs of a reversible transition matrix P by the same proportion, then adjusting the diagonal entries to make rows sum to 1, if possible, we get a new reversible transition matrix which has the same limiting probabilities as the original one.*

i.e. Let $p'_{i_0 j_0} = a p_{i_0 j_0}$ and $p'_{j_0 i_0} = a p_{j_0 i_0}$ for fixed $i_0, j_0 \in S$, and leave all other p_{ij} alone.

If the resulting matrix is P', then P' is reversible as well with the same limiting probability vector as P.

Proof. Consider a reversible Markov process $\{X\}$, and then a new process $\{X'\}$ can be obtained from X by modifying the transition rates between states i_0 and j_0 in symmetric pairs by a multiplicative factor

$$p'_{i_0 j_0} = a p_{i_0 j_0} \text{ and } p'_{j_0 i_0} = a p_{j_0 i_0}$$

Actually, we can do the symmetric modification as many times as one likes.

Kolmogorov's criterion implies that $\{X'\}$ is also reversible, since the all the path probability equations involving both i_0 and j_0 are changed in by exactly the same factor and hence still hold.

Further, the ratios of stationary distribution of $\{X'\}$ are exactly the same as those of $\{X\}$,

$$\text{since } \pi'_{i_0} p'_{i_0 j_0} = \pi'_{j_0} p'_{j_0 i_0}$$
$$\text{implies } \frac{\pi'_{i_0}}{\pi'_{j_0}} = \frac{p'_{j_0 i_0}}{p'_{i_0 j_0}} = \frac{a p_{ji}}{a p_{ij}} = \frac{p_{ji}}{p_{ij}} = \frac{\pi_i}{\pi_j},$$

which implies that the stationary distribution of $\{X'\}$ is identical to that of $\{X\}$. □

Example 5.1.1. *Suppose we have a Markov chain with transition matrix*

$$P = \begin{bmatrix} .25 & .25 & .25 & .25 \\ .3 & .1 & .3 & .3 \\ .15 & .15 & .55 & .15 \\ .1 & .1 & .1 & .7 \end{bmatrix},$$

and $S = \{1, 2, 3, 4\}$

This transition matrix is reversible since it has equal row entries, which follows from statements in previous chapter. We can compute the stationary distribution of this process by finding a large power of P. *Taking* P *to the power of 100, we get the limiting probabilities to be*

$$\pi = [0.1666667, 0.1388889, 0.2777778, 0.4166667]$$

Now we modify the symmetric pairs of this matrix.

We set $a_{12} = a_{21} = .5, a_{13} = a_{31} = 2,$ *and* $a_{24} = a_{42} = 1.5.$

Thus the new transition matrix is

$$P' = \begin{bmatrix} .125 & .125 & .5 & .25 \\ .15 & .1 & .3 & .45 \\ .3 & .15 & .4 & .15 \\ .1 & .15 & .1 & .65 \end{bmatrix},$$

which is obtained by setting $p'_{ij} = a_{ij}p_{ij}$*, and then adjusting the diagonal entries to ensure that the new matrix is in fact a probability transition matrix, i.e., row entries are nonnegative and sum to one.*

This new matrix P' *is reversible by Property 5.1.1. Taking* P' *to the power of 100, we get the limiting probabilities as*

$$\pi = (0.1666667, 0.1388889, 0.2777778, 0.4166667),$$

which gives the identical stationary distribution as that of the original process.

This symmetric transition probability scaling method can be considered as a natural consequence of Kolmogorov's criterion. Note that not all Markov processes have stationary distributions that are invariant to symmetric scaling of their transition rates, however for reversible processes this is always true.

5.2 Scale rows or columns except diagonal

Property 5.2.1. *By multiplying a row or column of a reversible transition matrix with a factor* $\alpha \neq 1$*, then adjusting the diagonal entry to make the matrix appropriate, we will get a new reversible transition matrix. But the stationary distribution changes.*

Proof. :

Consider a reversible Markov chain, with state space S, which is defined by transition matrix P. If we change the i-th row from p_{ij} to $p'_{ij} = \alpha p_{ij}$ for all $j \in S$, then any equation of Kolmogorov's criterion involving state i for the new matrix P' looks like

$$\begin{aligned} \cdots p_{ki} p'_{ij} p_{jl} \cdots &= \cdots p_{lj} p_{ji} p'_{ik} \cdots \\ \Leftrightarrow \cdots p_{ki} \alpha p_{ij} p_{jl} \cdots &= \cdots p_{lj} p_{ji} \alpha p_{ik} \cdots \\ \Leftrightarrow \cdots p_{ki} p_{ij} p_{jl} \cdots &= \cdots p_{lj} p_{ji} p_{ik} \cdots \end{aligned}$$

which is true by the Kolmogorov Criterion since the original transition matrix P is reversible. □

Example 5.2.1. *: Consider the transition matrix*

$$P = \begin{bmatrix} .45 & .3 & .15 & .1 \\ .25 & .5 & .15 & .1 \\ .25 & .3 & .35 & .1 \\ .25 & .3 & .15 & .3 \end{bmatrix},$$

which is reversible by Property (4.3.1) *since it has equal column entries except the diagonal. We compute its limiting probabilities and get*

$$\pi = (0.3125, 0.315, 0.1875, 0.125).$$

We modify this matrix by multiplying the row with a constant factor b_i with respect to ith row, and then adjust the diagonal entries to make the new transition matrix proper.

For instance we set $b_1 = 1.5, b_2 = 1.2, b_3 = .8$ and $b_4 = 1$, and adjust the diagonal *entries. We get a new transition matrix*

$$P' = \begin{bmatrix} .175 & .45 & .225 & .15 \\ .3 & .4 & .18 & .12 \\ .2 & .24 & .48 & .08 \\ .25 & .3 & .15 & .3 \end{bmatrix}.$$

We compute the limiting probabilities of P' and get

$$\pi' = (0.2366864, 0.3550296, 0.2662722, 0.1420118).$$

Compared to the first scaling method which remains invariant limiting probabilities, this second scaling method has different limiting probabilities after scaling. We are interested in how the limiting probabilities change. That is expresses in the following result which is new.

Property 5.2.2. *Let P be the transition matrix for reversible Markov Chain with n states and limiting probability vector $\underline{\pi} = (\pi_1, \ldots, \pi_i, \ldots, \pi_n)$. Modify P by multiplying row i by m and adjusting the diagonal such that the new matrix P' is still a transition matrix. Then the limiting vector of P' is*

$$\begin{aligned} \underline{\pi}' &= (\pi'_1, \ldots, \pi'_i, \ldots, \pi'_n) \\ &= (a\pi_1, \ldots, b\pi_i, \ldots, a\pi_n) \end{aligned}$$

where $a = \dfrac{m}{m + \pi_i(1-m)}$ and $b = \dfrac{1}{m + \pi_i(1-m)}$.

Proof. In the following, we assume that denominators are never zero and $i \neq 1$. If these assumptions are not satisfied, then the argument can be adjusted.

By Property 5.2.1, P' is reversible. By the detailed balance equations, we have

$$\frac{\pi'_i}{\pi'_1} = \frac{p'_{1i}}{p'_{i1}} = \frac{p_{1i}}{mp_{i1}} = (\frac{1}{m})\frac{p_{1i}}{p_{i1}} = (\frac{1}{m})\frac{\pi_i}{\pi_1}$$

Multiplying just row i by a constant will not change the ratios of the other limiting probabilities so

$$\begin{aligned}\underline{\pi}' &= (\pi_1', \ldots, \pi_i', \ldots, \pi_n') \\ &= (a\pi_1, \ldots, b\pi_i, \ldots, a\pi_n)\end{aligned}$$

and since the probabilities sum to 1, we have
$1 = (a(\pi_1 + \cdots + \pi_n - \pi_i) + b\pi_i) = a(1 - \pi_i) + b\pi_i$. Thus $a = \dfrac{1 - b\pi_i}{1 - \pi_i}$. Thus

$$\underline{\pi}' = (\frac{1 - b\pi_i}{1 - \pi_i}\pi_1, \ldots, b\pi_i, \ldots, \frac{1 - b\pi_i}{1 - \pi_i}\pi_n).$$

Hence

$$\frac{\pi_i'}{\pi_1'} = \frac{b\pi_i}{\left(\dfrac{1 - b_i\pi_i}{1 - \pi_i}\right)\pi_1} = \frac{b(1 - \pi_i)}{1 - b\pi i}\frac{\pi_i}{\pi_1} \text{ so } \frac{1}{m} = \frac{b(1 - \pi_i)}{1 - b\pi i}.$$

Solving for b and a gives $b = \dfrac{1}{m + \pi_i(1 - m)}$ and $a = \dfrac{m}{m + \pi_i(1 - m)}$.

□

To check the result, consider the following example.

Example 5.2.2.

Compose a reversible matrix

$$P = \begin{bmatrix} .4 & .2 & .4 \\ .45 & .1 & .45 \\ .2 & .1 & .7 \end{bmatrix}$$

P is reversible since it was composed initially from an equal row matrix with a one time symmetric pair scaling.

The limiting vector of P is

$$\underline{\pi} = [0.2903226, 0.1290323, 0.5806452]$$

We conduct a row scaling to the second row of P from .45 to .4 (i.e. take $m = 8/9$) and then adjust the diagonal entry from $p_{22} = .1$ to $p^*_{22} = .2$. According to Property 5.2.2, the new limiting probability of state 2 should be

$$\begin{aligned} \pi'_2 &= b\pi_2 = \tfrac{1}{m+\pi_2(1-m)}\pi_2 = \frac{.1290323}{8/9 + 1290323(1-8/9)} \\ &= 0.1428571 \end{aligned}$$

By computing in R, the limiting vector of P^* is

$$\underline{\pi^*} = [0.2857143, 0.1428571, 0.5714286]$$

which is consistent with the result.

Chapter 6

Product: symmetric and diagonal matrices

6.1 Product of symmetric and diagonal matrices

The following is taken from Kelly (1979). He does not present a proof and we provide one here.

Property 6.1.1. *A stationary Markov chain is reversible if and only if the matrix of transition probabilities can be written as the product of a symmetric and a diagonal matrix. i.e. P is the transition matrix for a reversible Markov chain iff $P = SD$ where S is a symmetric matrix and D a diagonal matrix such that $\sum_j p_{ij} = 1, \forall k$.*

Proof.

Part I: We show the necessity first. i.e. Let $P = SD$ where S is a symmetric matrix and D a diagonal matrix, be such that $\sum_j p_{ij} = 1, \forall k$. We will show that P is a reversible transition matrix.

$$\text{Let } P = SD = \begin{bmatrix} s_{11} & s_{12} & s_{13} & \cdots \\ s_{21} & s_{22} & s_{23} & \cdots \\ s_{31} & s_{32} & s_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} d_{11} & 0 & 0 & \cdots \\ 0 & d_{22} & 0 & \cdots \\ 0 & 0 & d_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix}$$

$$= \begin{bmatrix} s_{11}d_{11} & s_{12}d_{22} & s_{13}d_{33} & \cdots \\ s_{21}d_{11} & s_{22}d_{22} & s_{23}d_{33} & \cdots \\ s_{31}d_{11} & s_{32}d_{22} & s_{33}d_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix}.$$

Then

$$(d_{11}, d_{22}, d_{33}, \cdots)P$$

$$= (d_{11}, d_{22}, d_{33}, \cdots) \begin{bmatrix} s_{11}d_{11} & s_{12}d_{22} & s_{13}d_{33} & \cdots \\ s_{21}d_{11} & s_{22}d_{22} & s_{23}d_{33} & \cdots \\ s_{31}d_{11} & s_{32}d_{22} & s_{33}d_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix}$$

$$= (s_{11}d_{11}^2 + s_{21}d_{22}d_{11} + s_{31}d_{33}d_{11} + \cdots, s_{12}d_{11}d_{22} + s_{22}d_{22}^2 + s_{32}d_{33}d_{22} + \cdots, \cdots)$$

$$= (d_{11}(s_{11}d_{11} + s_{21}d_{22} + s_{31}d_{33}) + \cdots, d_{22}(s_{12}d_{11} + s_{22}d_{22} + s_{32}d_{33} + \cdots), \cdots)$$

$$= (d_{11}(s_{11}d_{11} + s_{12}d_{22} + s_{13}d_{33}) + \cdots, d_{22}(s_{21}d_{11} + s_{22}d_{22} + s_{23}d_{33} + \cdots), \cdots)$$

$$= (d_{11}\sum_j p_{1j}, d_{22}\sum_j p_{1j}, \ldots) = (d_{11}, d_{22}, \ldots).$$

Thus we have

$$(d_{11}d_{22}d_{33}\cdots)P = (d_{11}d_{22}d_{33}\cdots).$$

Rewrite this as

$$\frac{1}{\sum_k d_{kk}}(d_{11}d_{22}d_{33}\cdots)P = \frac{1}{\sum_k d_{kk}}(d_{11}d_{22}d_{33}\cdots).$$

We know that the limiting probability is the solution of $\underline{\pi}P = \underline{\pi}$. Together with the uniqueness of stationary distribution, we conclude that

$$\underline{\pi} = (\frac{d_{11}}{\sum_k d_{kk}}, \frac{d_{22}}{\sum_k d_{kk}}, \frac{d_{22}}{\sum_k d_{kk}}, \cdots).$$

Further, we have

$$\pi_i p_{ij} = \frac{d_{ii}}{\sum_k d_{kk}} s_{ij} d_{jj}$$

since $\{p_{ij}\} = \{s_{ij}d_{jj}\}$. Thus, since $s_{ij} = s_{ji}$, we get

$$\pi_j p_{ji} = \frac{d_{jj}}{\sum_k d_{kk}} s_{ji} d_{ii} = \pi_i p_{ij}.$$

Thus we get the detailed balance equations for the Markov chain defined by $P = SD$. Therefore the Markov chain is reversible.

Part II: We next prove the sufficiency.

Let P be transition matrix of a reversible Markov chain. We will show that P can be written as a product of a symmetric matrix (S) and a diagonal matrix (D), i.e., $P = SD$.

Take $D = \begin{bmatrix} \pi_1 & 0 & 0 & \cdots \\ 0 & \pi_2 & 0 & \cdots \\ 0 & 0 & \pi_3 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix}$

Then take

$$\begin{aligned} S &= PD^{-1} \\ &= \begin{bmatrix} p_{11} & p_{12} & p_{13} & \cdots \\ p_{21} & p_{22} & p_{23} & \cdots \\ p_{31} & p_{32} & p_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} \frac{1}{\pi_1} & 0 & 0 & \cdots \\ 0 & \frac{1}{\pi_2} & 0 & \cdots \\ 0 & 0 & \frac{1}{\pi_3} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \end{aligned}$$

$$= \begin{bmatrix} \frac{p_{11}}{\pi_1} & \frac{p_{12}}{\pi_2} & \frac{p_{13}}{\pi_3} & \dots \\ \frac{p_{21}}{\pi_1} & \frac{p_{22}}{\pi_2} & \frac{p_{23}}{\pi_3} & \dots \\ \frac{p_{31}}{\pi_1} & \frac{p_{32}}{\pi_2} & \frac{p_{33}}{\pi_3} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

We know $\pi_i p_{ij} = \pi_j p_{ji}$, since the Markov chain is reversible.

Thus we get

$$S = \begin{bmatrix} \frac{p_{11}}{\pi_1} & \frac{p_{21}}{\pi_1} & \frac{p_{31}}{\pi_1} & \dots \\ \frac{p_{21}}{\pi_1} & \frac{p_{22}}{\pi_2} & \frac{p_{32}}{\pi_2} & \dots \\ \frac{p_{31}}{\pi_1} & \frac{p_{32}}{\pi_2} & \frac{p_{33}}{\pi_3} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

which is clearly a symmetric matrix. Since $S = PD^{-1}$, we get $P = SD$, as required.

□

Example 6.1.1. *:*

Let

$$P = \begin{bmatrix} .4 & .3 & .3 \\ .4 & .2 & .4 \\ .6 & .2 & .2 \end{bmatrix}$$

P is a reversible transition matrix since it has equal row entries.

We calculate out its limiting probability as

$$\underline{\pi} = [0.4590164, 0.2459016, 0.2950820]$$

Let D be a diagonal matrix with $\{\pi_i\}$ as its diagonal entries. Then let

$$\begin{aligned} S &= PD^{-1} \\ &= \begin{bmatrix} .4 & .3 & .3 \\ .4 & .2 & .4 \\ .2 & .2 & .6 \end{bmatrix} \begin{bmatrix} 3.25 & 0 & 0 \\ 0 & 4.333334 & 0 \\ 0 & 0 & 2.166666 \end{bmatrix} \end{aligned}$$

$$= \begin{bmatrix} 1.30 & 1.3000002 & 0.6499999 \\ 1.30 & 0.8666668 & 0.8666666 \\ 0.65 & 0.8666668 & 1.2999999 \end{bmatrix}$$

Note 1. *The above result is obtained by R. Here we can see S is a symmetric matrix (with reasonable tolerance on accuracy).*

Example 6.1.2. *:*

Let S be any arbitrary symmetric matrix, and D be any arbitrary diagonal matrix, for instance

$$\begin{aligned} P = SD &= \begin{bmatrix} 2 & 1 & 3 \\ 1 & 3 & 4 \\ 3 & 4 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \\ &= \begin{bmatrix} 2 & 2 & 9 \\ 1 & 6 & 12 \\ 3 & 8 & 6 \end{bmatrix} \end{aligned}$$

Using our previous scaling methodology, we modify P to be a proper transition matrix P'

$$P' = \begin{bmatrix} \frac{2}{13} & \frac{2}{13} & \frac{9}{13} \\ \frac{1}{19} & \frac{6}{19} & \frac{12}{19} \\ \frac{3}{17} & \frac{8}{17} & \frac{8}{17} \end{bmatrix}$$

We can check whether P' is reversible by using the method in chapter 1.

Let $A = P\prime^{100}$ and calculate $A^T P'$, we get

$$A^T P' = \begin{bmatrix} 0.01960784 & 0.01960784 & 0.0882353 \\ 0.01960784 & 0.11764706 & 0.2352941 \\ 0.08823529 & 0.23529412 & 0.1764706 \end{bmatrix}$$

which is symmetric. Thus P' is a reversible transition matrix constructed from the product of a symmetric matrix and a diagonal matrix.

As an application of this method, see Richman and Sharp (1990).

Chapter 7

Graph Method

7.1 Graph Method

Property 7.1.1. *:*

Consider an arbitrarily connected graph. A link between vertices i and j has weight w_{ij}, with $w_{ji} = w_{ij}, i, j \in S$. Define the transition probabilities of a Markov chain by $p_{ij} = \frac{w_{ij}}{\sum_k w_{kk}}$. Then the Markov chain is reversible.

Proof. :
We guess that $\pi_i = \frac{\sum_k w_{ik}}{\sum_l \sum_k w_{lk}}, i, l, k \in S.$
We interpret this as the proportion of time that the system is in state i, i.e., the stationary probability of staying in state i.

It is easy to check that $\sum_i \pi_i = \frac{\sum_i \sum_k w_{ik}}{\sum_l \sum_k w_{lk}} = 1.$

We find that

$$\pi_i p_{ij} = \frac{\sum_k w_{ik}}{\sum_l \sum_k w_{lk}} \cdot \frac{w_{ij}}{\sum_k w_{ik}} = \frac{w_{ij}}{\sum_l \sum_k w_{lk}}.$$

Similarly,

$$\pi_j p_{ji} = \frac{\sum_k w_{jk}}{\sum_l \sum_k w_{lk}} \cdot \frac{w_{ji}}{\sum_k w_{jk}} = \frac{w_{ji}}{\sum_l \sum_k w_{lk}} = \frac{w_{ij}}{\sum_l \sum_k w_{lk}} = \pi_i p_{ij},$$

since $w_{ij} = w_{ji}$.

Further, we have shown that our guess and interpretation of π_i is correct since the stationary distribution is unique.

Thus we conclude that a Markov chain defined in such a way is reversible with $\{\pi_i\}$ being the limiting probabilities. □

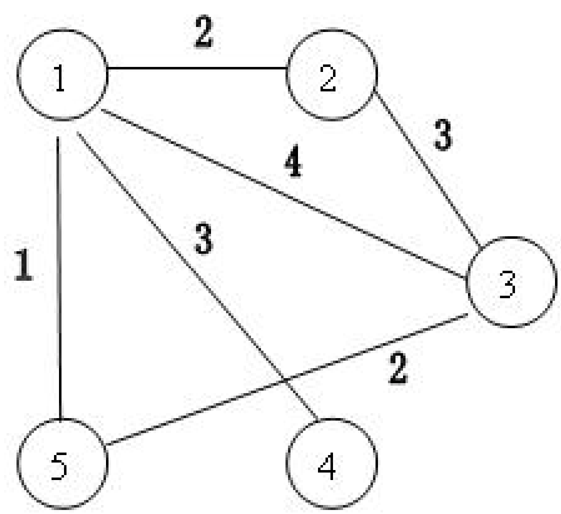

Figure 7.1: Graph with nodes

Example 7.1.1.

We assign numbers to the w_i in the graph as in Figure 7.1.

We write down a matrix by putting the weight numbers in the appropriate places.

$$W = \begin{bmatrix} 0 & 2 & 4 & 3 & 1 \\ 2 & 0 & 3 & 0 & 0 \\ 4 & 3 & 0 & 0 & 2 \\ 3 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 \end{bmatrix}$$

Obviously W is a symmetric matrix.

Next we scale the rows of W to convert it to a proper transition matrix P.

$$P = \begin{bmatrix} 0 & \frac{2}{10} & \frac{4}{10} & \frac{3}{10} & \frac{1}{10} \\ \frac{2}{5} & 0 & \frac{3}{5} & 0 & 0 \\ \frac{4}{9} & \frac{3}{9} & 0 & 0 & \frac{2}{9} \\ \frac{3}{3} & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & \frac{2}{3} & 0 & 0 \end{bmatrix}.$$

By Property 7.1.1, P is reversible and the limiting probability of state i is $\pi_i = \frac{\sum_k w_{ik}}{\sum_l \sum_k w_{lk}}$. So

$$\pi_1 = \frac{2+4+3+1}{(2+4+3+1)+(2+3)+(3+4+2)+3+(1+2)} = \frac{1}{3}.$$

Similarly

$$\pi_2 = \frac{1}{6}, \pi_3 = \frac{3}{10}, \pi_4 = \frac{1}{10}, \pi_5 = \frac{1}{10}.$$

We check the validity of limiting probabilities first.

Again using the limiting probability calculation method in chapter 1, we get

$$\pi_1 = 0.3333333, \pi_2 = 0.1666667, \pi_3 = 0.3, \pi_4 = 0.1, \pi_5 = 0.1$$

which is consistent with the above results.

Then check the reversibility by computing $(P^{100})^T P$,

$$(P^{100})^T P = \begin{bmatrix} 0 & 0.06666667 & 0.13333333 & 0.1 & 0.03333333 \\ 0.06666667 & 0 & 0.1 & 0 & 0 \\ 0.13333333 & 0.1 & 0 & 0 & 0.06666667 \\ 0.1 & 0 & 0 & 0 & 0 \\ 0.03333333 & 0 & 0.06666667 & 0 & 0 \end{bmatrix}$$

Since the resulting matrix is symmetric, the Markov chain with transition matrix P is reversible.

Chapter 8

Tree Process

8.1 Definition

The following is from to Ross (2007).

Definition: "A Markov chain is said to be a tree process if

(i) $p_{ij} > 0$ whenever $p_{ji} > 0$,

(ii) for every pair of states i and j, $i \neq j$,

there is a unique sequence of distinct states $i = i_0, i_1, i_2, \cdots, i_{n-1}, i_n = j$ such that

$$p_{i_k i_{k-1}} > 0, \qquad k = 0, 1, 2, \cdots, n-1$$

In other words, a Markov chain is a tree process if for every pair of distinct states i and j, there is a unique way for the process to go from i to j without reentering a state (and this path is the reverse of the unique path form j to i)."

Graphically, the tree structure is a structure of the type shown in Figure 8.1, where nodes stand for states.

The following is from Ross (2007).

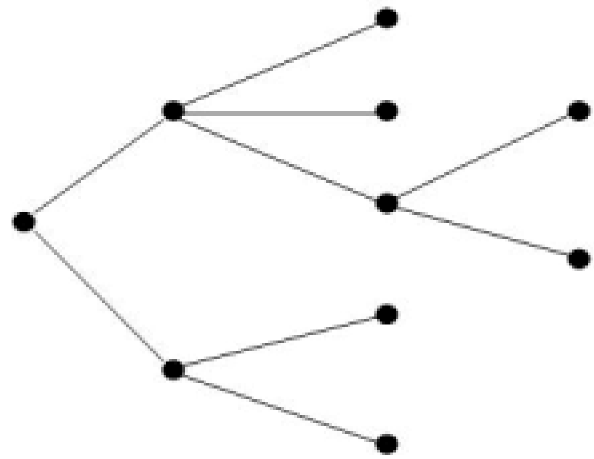

Figure 8.1: Tree structure

Property 8.1.1.

An ergodic tree process is reversible.

Proof.

By the definition of a tree process, from state i to state j, there is a unique path. From j to i, there is also a unique path and this path is the reverse of the path from i to j. Thus, for any path, the Kolmogorov's condition is undoubtedly satisfied. For example, if there is a path from state i to state j via states k and l, then Kolmogorov's condition is

$$p_{ik}p_{kl}p_{lj}p_{jl}p_{lk}p_{ki} = p_{ik}p_{kl}p_{lj}p_{jl}p_{lk}p_{ki}.$$

Both sides of the equation are exactly the same.

Intuitively, a tree structure must have detailed (local) balance. □

8.2 Example

Example 8.2.1.

We are given a tree structure as in Figure 8.2.1.

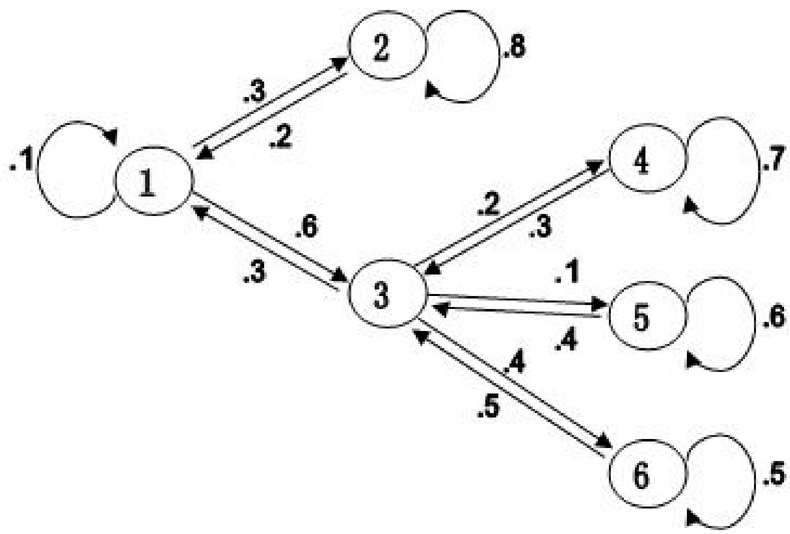

Figure 8.2: Tree structure example

We write down its transition matrix

$$P = \begin{bmatrix} .1 & .3 & .6 & 0 & 0 & 0 \\ .2 & .8 & 0 & 0 & 0 & 0 \\ .3 & 0 & 0 & .2 & .1 & .4 \\ 0 & 0 & .3 & .7 & 0 & 0 \\ 0 & 0 & .4 & 0 & .6 & 0 \\ 0 & 0 & .5 & 0 & 0 & .5 \end{bmatrix}$$

We check the reversibility of P by using the methods in chapter 1.

Firstly calculate the limiting probability of P to be $\pi_1 = 0.126050, \pi_2 = 0.189076,$ $\pi_3 = 0.252101, \pi_4 = 0.168067, \pi_5 = 0.0630252, \pi_6 = 0.201681.$

excluding

Then check the reversibility by computing $(P^{100})^T P$,

$$(P^{100})^T P = \begin{bmatrix} 0.01 & 0.06 & 0.18 & 0.00 & 0.00 & 0.00 \\ 0.06 & 0.64 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.18 & 0.00 & 0.00 & 0.06 & 0.04 & 0.20 \\ 0.00 & 0.00 & 0.06 & 0.49 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.04 & 0.00 & 0.36 & 0.00 \\ 0.00 & 0.00 & 0.20 & 0.00 & 0.00 & 0.25 \end{bmatrix}$$

Since $(P^{100})^T P$ *is a symmetric matrix, we conclude that the tree process is reversible.*

Chapter 9

Triangular completion method

9.1 Algorithm

1. We are given $\underline{\pi}$ (or choose $\underline{\pi}$).

2. Choose probabilities for the upper triangular part (or lower triangular part), excluding diagonals.

3. Calculate the lower triangular entries by the detailed balance equations of a reversible process,

   e.g.,

$$\pi_2 p_{21} = \pi_1 p_{12}.$$

$$p_{21} = \frac{\pi_1 p_{12}}{\pi_2}.$$

4. If row entries sum to less than (or equal to) 1, then set the diagonal entry so that the row sums to 1. If a row has entries that sum to more than 1, scale the row to make it sum to less than (or equal to) 1 and then set the diagonal entry as in the previous case.

We have not seen this algorithm explicitly stated.

Property 9.1.1. *The triangular completion method makes a reversible transition matrix with a given limiting probability.*

Proof.

Since we calculate the lower triangular entries from the detailed balance equation, we have

$$\pi_i p_{ij} = \pi_j p_{ji} \qquad \forall i, j$$

where either p_{ij} or p_{ji} is given and the other is computed.

Then we have

$$\pi_i p_{ii_0} \pi_{i_0} p_{i_0 i_1} \cdots \pi_{i_n} p_{i_n i} = \pi_i p_{ii_n} \pi_{i_n} p_{i_n i_{n-1}} \cdots \pi_{i_0} p_{i_0 i}.$$

Cancel out the $\pi' s$ to get

$$p_{ii_0} p_{i_0 i_1} \cdots p_{i_n i} = p_{ii_n} p_{i_n i_{n-1}} \cdots p_{i_0 i}. \tag{9.1}$$

One thing that should be noted is that the computed entries are not necessarily a probabilities since they are quite possibly greater than 1. But Equation (9.1) is always true and we can scale the row (by multiplying by a constant less than 1) to make sure that we have a valid transition matrix. Then Kolmogorov's criterion is satisfied so the resulting matrix is reversible. □

9.2 Example

Example 9.2.1.

Step 1. We are given $\underline{\pi} = (.2, .1, .5, .2)$

Step 2. Choose the upper triangular part, leaving the diagonal blank. Let

$$P = \begin{bmatrix} \_ & .2 & .1 & .4 \\ p_{21} & \_ & .3 & .5 \\ p_{31} & p_{32} & \_ & .8 \\ p_{41} & p_{42} & p_{43} & \_ \end{bmatrix}$$

Step 3. Calculate the lower triangular entries, i.e., the p_{ij}'s $(i > j)$, using the detailed balance equations of a reversible process.

$$\pi_2 p_{21} = \pi_i p_{12}$$

$$p_{21} = \frac{\pi_1 p_{12}}{\pi_2} = \frac{.2(.2)}{.1} = .4$$

Similarly we get other p's and the matrix P.

$$P = \begin{bmatrix} \_ & .2 & .1 & .4 \\ .4 & \_ & .3 & .5 \\ .04 & .06 & \_ & .8 \\ .4 & .25 & 2 & \_ \end{bmatrix}.$$

Step 4. Since the second row and the fourth row both sum to more than one, we have to scale them. We multiply row two by $\times 0.5$ (for example) and row four by $\times 0.25$. Then we fill in the diagonal entries to make a valid transition matrix.

$$P' = \begin{bmatrix} .3 & .2 & .1 & .4 \\ .2 & .4 & .15 & .25 \\ .04 & .06 & .1 & .8 \\ .1 & .0625 & .5 & .3375 \end{bmatrix}.$$

Now we check the reversibility of the transition matrix P' using the method of Section 1.2.2.

We get limiting vector by raising P' to the 100th power. The result (row 1) is

$$\underline{\pi} = (0.1176471, 0.1176471, 0.2941176, 0.4705882).$$

Then

$$(P'^{100})^T * P' = \begin{bmatrix} 0.03529412 & 0.02352941 & 0.01176471 & 0.04705882 \\ 0.02352941 & 0.04705882 & 0.01764706 & 0.02941176 \\ 0.01176471 & 0.01764706 & 0.02941176 & 0.23529412 \\ 0.04705882 & 0.02941176 & 0.23529412 & 0.15882353 \end{bmatrix}$$

Since the above is a symmetric matrix, this verifies that P' is a transition matrix of a reversible Markov process.

We note in the example, that the limiting vector changes, i.e., it is no longer the limiting vector we start with. The reason is that we did a scaling adjustment to get the final transition matrix. The ratio of transition probabilities change, and thus the limiting probabilities change. We have discussed how the limiting probabilities change in Property 5.2.2.

Chapter 10

Convex Combination

10.1 Weighted Average

Property 10.1.1.

The convex combination of two reversible Markov transition matrices with the same stationary distribution $\underline{\pi}$, is reversible, and the stationary distribution remains the same.

Proof.

Let $A = \{a_{ij}\}$ and $B = \{b_{ij}\}$ be the transition matrices of two reversible processes. Let P be a convex combination of A and B.

$$P = \alpha A + (1 - \alpha)B, \qquad \alpha \in [0, 1].$$

Then P is a transition matrix since

$$\sum_j p_{ij} = \alpha \sum_j a_{ij} + (1 - \alpha) \sum_j b_{ij} = 1$$

Further,

$$\underline{\pi}P = \underline{\pi}(\alpha A + (1 - \alpha)B) = \alpha\underline{\pi}A + (1 - \alpha)\underline{\pi}B = \alpha\underline{\pi} + (1 - \alpha)\underline{\pi} = \underline{\pi},$$

$$\begin{aligned} \pi_i p_{ij} &= \alpha\pi_i a_{ij} + (1-\alpha)\pi_i b_{ij} \\ &= \alpha\pi_j a_{ji} + (1-\alpha)\pi_j b_{ji}, \text{ since } A \text{ and } B \text{ are reversible} \\ &= \pi_j(\alpha a_{ji} + (1-\alpha) b_{ji}) \\ &= \pi_j p_{ji}. \end{aligned}$$

Thus, P is reversible. □

10.2 Example

Example 10.2.1. *We will use the examples from section 5.1 on the Symmetric Pairs Scaling method.*

$$A = \begin{bmatrix} .25 & .25 & .25 & .25 \\ .3 & .1 & .3 & .3 \\ .15 & .15 & .55 & .15 \\ .1 & .1 & .1 & .7 \end{bmatrix},$$

and

$$B = \begin{bmatrix} .125 & .125 & .5 & .25 \\ .15 & .1 & .3 & .45 \\ .3 & .15 & .4 & .15 \\ .1 & .15 & .1 & .65 \end{bmatrix},$$

A and B have the same limiting vector

$$\underline{\pi} = (0.1666667, 0.1388889, 0.2777778, 0.4166667)$$

Let P be the convex combination of A and B,

$$P = 0.3 * A + 0.7 * B$$

$$= \begin{bmatrix} 0.1625 & 0.1625 & 0.425 & 0.250 \\ 0.1950 & 0.1000 & 0.300 & 0.405 \\ 0.2550 & 0.1500 & 0.445 & 0.150 \\ 0.1000 & 0.1350 & 0.100 & 0.665 \end{bmatrix}$$

We now find out the limiting vector of P and check its reversibility using the method from Section 1.2.2.

Calculating P^{100}, we get the limiting vector of P as

$$\underline{\pi} = (0.1666667, 0.1388889, 0.2777778, 0.4166667),$$

and

$$(P^{100})^T * P = \begin{bmatrix} 0.02708333 & 0.02708333 & 0.07083333 & 0.04166667 \\ 0.02708333 & 0.01388889 & 0.04166667 & 0.05625000 \\ 0.07083333 & 0.04166667 & 0.12361111 & 0.04166667 \\ 0.04166667 & 0.05625000 & 0.04166667 & 0.27708333 \end{bmatrix}.$$

This is symmetric, and verifies that P, the convex combination of two reversible matrices, is reversible.

Corollary 10.3. *The convex combination of a countable collection of reversible matrices is reversible, i.e.,*

$$P = \alpha_0 P_0 + \alpha_1 P_1 + \alpha_2 P_2 + \alpha_3 P_3 + \cdots$$

is reversible, where

i) $\{P_i\}, i = 0, 1, 2, 3, \cdots$ *are reversible Markov transition matrices, and*

ii) $\sum_i \alpha_i = 1, 1 \geq \alpha_i \geq 0.$

Chapter 11

Reversibility and Invariance

The following two properties are stated (without proof) and are taken from Strook (2005). The proofs given are ours. Let P be the transition matrix of a Markov chain. Let P^* be the transition matrix for the reversed Markov chain. It is know that both matrices have the same limiting vector. The limiting vector of P is invariant under the construction of the two reversible transition matrices in the next two properties.

11.1 $\frac{P+P^*}{2}$

Property 11.1.1. *Let P be any transition matrix with limiting vector $\underline{\pi}$. Define $P^* = \{q_{ij}\}$ where $q_{ij} = \frac{\pi_j}{\pi_i} p_{ji}$. Then $\frac{P+P^*}{2}$ is reversible with limiting vector$\underline{\pi}$.*

Proof.

First P and P^* have the same limiting probabilities.

A weighted average of two transition matrices with the same limiting probability vector is a transition matrix with the same limiting probability vector.

Let $M = [m_{ij}] = \frac{P+P^*}{2} = [\frac{p_{ij}}{2} + \frac{\pi_j}{2\pi_i}p_{ji}]$. Clearly

$$m_{ij} = \frac{p_{ij}}{2} + \frac{\pi_j}{2\pi_i}p_{ji} \geq 0.$$

Then

$$\begin{aligned}\sum_j m_{ij} &= \sum_j \frac{p_{ij}}{2} + \sum_j \frac{\pi_j}{2\pi_i}p_{ji} \\ &= \frac{1}{2}\sum_j p_{ij} + \frac{1}{2\pi_i}\sum_j \pi_j p_{ji} \\ &= \frac{1}{2} + \frac{\pi_i}{2\pi_i} \\ &= 1\end{aligned}$$

where

$$\sum_j \pi_j p_{ji} = \pi_i, \text{ since } \underline{\pi}P = \underline{\pi}.$$

Thus, $\frac{P+P^*}{2}$ is a transition matrix.

Further, by the definition of P^*, it is the transition matrix of the reversed process defined by P. So P^* has the same stationary distribution as P. So

$$\underline{\pi}M = \frac{\underline{\pi}P + \underline{\pi}P^*}{2} = \frac{\pi + \pi}{2} = \underline{\pi}.$$

Lastly, we check the detailed balance equations for $\frac{P+P^*}{2}$.

$$\begin{aligned}\pi_i m_{ij} &= \pi_i(\frac{p_{ij}}{2} + \frac{\pi_j}{2\pi_i}p_{ji}) \\ &= \frac{1}{2}(\pi_i p_{ij} + \pi_j p_{ji}) \\ &= \pi_j(\frac{\pi_i}{2\pi_j}p_{ij} + \frac{p_{ji}}{2}) \\ &= \pi_j m_{ji}.\end{aligned}$$

Therefore, we can conclude that $\frac{P+P^*}{2}$ is a transition matrix defined by a reversible Markov process which has $\underline{\pi}$ as its limiting probability. □

Example 11.1.1. *Consider a transition matrix*

$$P = \begin{bmatrix} .2 & .4 & .4 \\ .3 & .2 & .5 \\ .3 & .3 & .4 \end{bmatrix},$$

which has limiting vector as $\underline{\pi} = [\frac{33}{121}, \frac{36}{121}, \frac{52}{121}]$. *We can check that* P *is not reversible.*

Then we construct another transition matrix $P^* = \{q_{ij}\}$ *by the rule* $q_{ij} = \frac{\pi_j}{\pi_i} p_{ji}$:

$$P^* = \begin{bmatrix} \frac{1}{5} & \frac{18}{55} & \frac{26}{55} \\ \frac{11}{30} & \frac{1}{5} & \frac{13}{30} \\ \frac{33}{130} & \frac{45}{130} & \frac{2}{5} \end{bmatrix}.$$

Thus we get the following result using R:

$$\frac{P+P^*}{2} = \begin{bmatrix} 0.2000000 & 0.3636364 & 0.4363636 \\ 0.3333333 & 0.2000000 & 0.4666667 \\ 0.2769231 & 0.3230769 & 0.4000000 \end{bmatrix}.$$

The limiting vector of $\frac{P+P^*}{2}$ *is*

$$(\frac{P+P^*}{2})^{100} = \begin{bmatrix} 0.2727273 & 0.2975207 & 0.4297521 \\ 0.2727273 & 0.2975207 & 0.4297521 \\ 0.2727273 & 0.2975207 & 0.4297521 \end{bmatrix},$$

and checking the reversibility of $\frac{P+P^*}{2}$ *we get*

$$((\frac{P+P^*}{2})^{100})^T * \frac{P+P^*}{2} = \begin{bmatrix} 0.05454545 & 0.09917355 & 0.1190083 \\ 0.09917355 & 0.05950413 & 0.1388430 \\ 0.11900826 & 0.13884298 & 0.1719008 \end{bmatrix}$$

We see that $\frac{P+P^*}{2}$ *is a reversible transition matrix which has the same limiting vector as* P.

11.2 P^*P

Property 11.2.1. *Let P be any transition matrix with limiting vector $\underline{\pi}$. Define $P^* = \{q_{ij}\}$ where $q_{ij} = \frac{\pi_j}{\pi_i} p_{ji}$. Then P^*P is reversible with the same limiting probability vector as P.*

Proof.

First, the product of two transition matrices is a transition matrix, since it represents a two step transition with two different matrices. If $\underline{\pi}$ is the limiting vector for P, then $\underline{\pi}$ is also the limiting vector for P^* since P^* is the transition matrix for the reverse Markov chain.

Let $R = P^*P$. Then

$$\begin{aligned}\sum_j r_{ij} &= \sum_j \sum_k q_{ik} p_{kj} \\ &= \sum_k \sum_j q_{ik} p_{kj} \\ &= \sum_k q_{ik} \sum_j p_{kj} \\ &= \sum_k q_{ik} = 1.\end{aligned}$$

Further,

$$\underline{\pi} P^* P = \underline{\pi} P = \underline{\pi}.$$

Then

$$\begin{aligned}\pi_i r_{ij} &= \pi_i \sum_k q_{ik} p_{kj} \\ &= \pi_i \sum_k \frac{\pi_k}{\pi_i} p_{ki} p_{kj} \\ &= \pi_j \sum_k \frac{\pi_k}{\pi_j} p_{kj} p_{ki} \\ &= \pi_j \sum_k q_{jk} p_{ki} = \pi_j r_{ji}.\end{aligned}$$

So P^*P is a reversible transition matrix with same limiting vector as P. □

Example 11.2.1. *We again use the P and P^* of our last example.*

$$P = \begin{bmatrix} .2 & .4 & .4 \\ .3 & .2 & .5 \\ .3 & .3 & .4 \end{bmatrix} \qquad \text{and} \qquad P^* = \begin{bmatrix} \frac{1}{5} & \frac{18}{55} & \frac{26}{55} \\ \frac{11}{30} & \frac{1}{5} & \frac{13}{30} \\ \frac{33}{130} & \frac{45}{130} & \frac{2}{5} \end{bmatrix}.$$

Then

$$P^*P = \begin{bmatrix} 0.2800000 & 0.2872727 & 0.4327273 \\ 0.2633333 & 0.3166667 & 0.4200000 \\ 0.2746154 & 0.2907692 & 0.4346154 \end{bmatrix}.$$

The limiting probability of P^*P is calculated as

$$(P^*P)^{100} = \begin{bmatrix} 0.2727273 & 0.2975207 & 0.4297521 \\ 0.2727273 & 0.2975207 & 0.4297521 \\ 0.2727273 & 0.2975207 & 0.4297521 \end{bmatrix},$$

and checking the reversibility of P^*P using Section 1.2.2 yields

$$((P^*P)^{100})^T * (P^*P) = \begin{bmatrix} 0.07636364 & 0.07834711 & 0.1180165 \\ 0.07834711 & 0.09421488 & 0.1249587 \\ 0.11801653 & 0.12495868 & 0.1867769 \end{bmatrix}$$

We can find that P^*P is reversible and has the same limiting vector as transition matrix P.

This chapter shows interesting methods which allow us to construct reversible matrices from non-reversible matrices and still retain the same stationary distribution.

Chapter 12

Expand and Merge Methods

12.1 State by State Expand

Property 12.1.1. *Given an $n \times n$ reversible Markov transition matrix P, we can expand it to an $(n+1) \times (n+1)$ reversible Markov transition matrix Q by setting the proper transition rates.*

We show this method with an example.

Example 12.1.1. *We begin with P, the transition matrix of a reversible Markov chain with 3 states.*

$$P = \begin{bmatrix} .5 & .3 & .2 \\ .3 & .3 & .4 \\ .1 & .2 & .7 \end{bmatrix}$$

We want to expand it by one more state to get a 4×4 transition matrix.

We expand P while leaving the diagonal blank.

$$Q = \begin{bmatrix} \_ & .3 & .2 & q_{14} \\ .3 & \_ & .4 & q_{24} \\ .1 & .2 & \_ & q_{34} \\ q_{41} & q_{42} & q_{43} & \_ \end{bmatrix}$$

Choose any symmetric pair of unknown q_{ij}'s arbitrarily, the ratios between rest of the pairs are forced. For instance, if we choose $q_{14} = .4$ and $q_{41} = .2$, then

$$\frac{q_{42}}{q_{24}} = \frac{\pi_2}{\pi_4} = \frac{\pi_2}{\pi_1}\frac{\pi_1}{\pi_4} = \frac{q_{12}}{q_{21}}\frac{q_{41}}{q_{14}} = \frac{.3}{.3}\frac{.2}{.4} = \frac{1}{2},$$

and similarly,

$$\frac{q_{43}}{q_{34}} = \frac{1}{1}.$$

Since we get all the ratios of symmetric pairs, we can compose Q in an infinite number of ways, with the help of scaling of course.

For instance, choose

$$Q = \begin{bmatrix} .1 & .3 & .2 & .4 \\ .15 & .35 & .2 & .3 \\ .1 & .2 & .3 & .4 \\ .2 & .3 & .4 & .1 \end{bmatrix}$$

Using the method in Section 1.2.2, to check for reversibility, we find

$$(Q^{100})^T * Q = \begin{bmatrix} 0.01428571 & 0.04285714 & 0.02857143 & 0.05714286 \\ 0.04285714 & 0.10000000 & 0.05714286 & 0.08571429 \\ 0.02857143 & 0.05714286 & 0.08571429 & 0.11428571 \\ 0.05714286 & 0.08571429 & 0.11428571 & 0.02857143 \end{bmatrix}.$$

The symmetry means that Q is reversible.

Actually, we do not need to bother checking for reversibility, since the symmetric pairs of Q satisfy the detailed balance equations.

12.2 Merge Method

This is our last method to construct transition matrices of reversible Markov chains. Yet it is the most expandable since it can glue any number of reversible Markov processes together to form a new reversible process which has a larger state space.

We demonstrate this method with an example first.

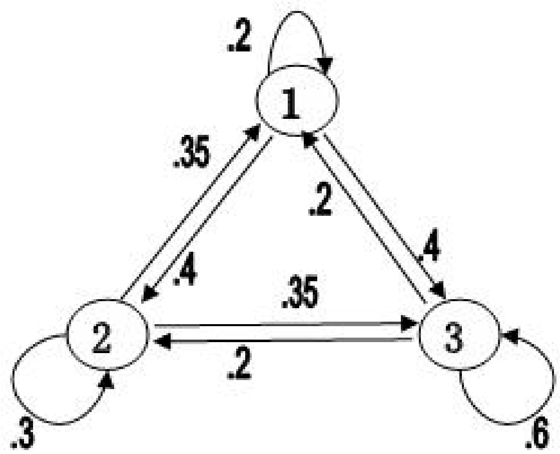

Figure 12.1: Process A

Example 12.2.1.

We are given two reversible processes which have A and B as their transition matrix respectively.

$$A = \begin{bmatrix} .2 & .4 & .4 \\ .35 & .3 & .35 \\ .2 & .2 & .6 \end{bmatrix}$$

and

$$B = \begin{bmatrix} .2 & .3 & .3 & .2 \\ .2 & .4 & .2 & .2 \\ .1 & .1 & .7 & .1 \\ .2 & .3 & .3 & .2 \end{bmatrix}.$$

Graphically, processes A and B can be shown as in Figure 12.2 and Figure 12.2.1.

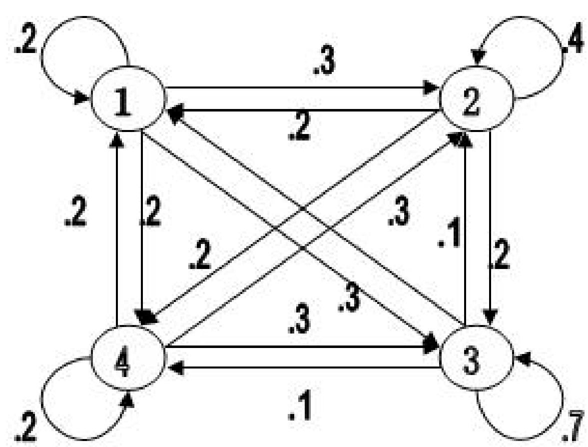

Figure 12.2: Process B

If we glue these two processes at state 3 *of Process A and state* 1 *of Process B, the combination graph would be shown in Figure 12.3.*

Then what will the new transition matrix be like?

Since the ratios between all transition probabilities are not affected by the merge, we keep the p_{ij}'s remaining the same and leave the diagonal entry of knot state, p_{33}, blank temporarily.

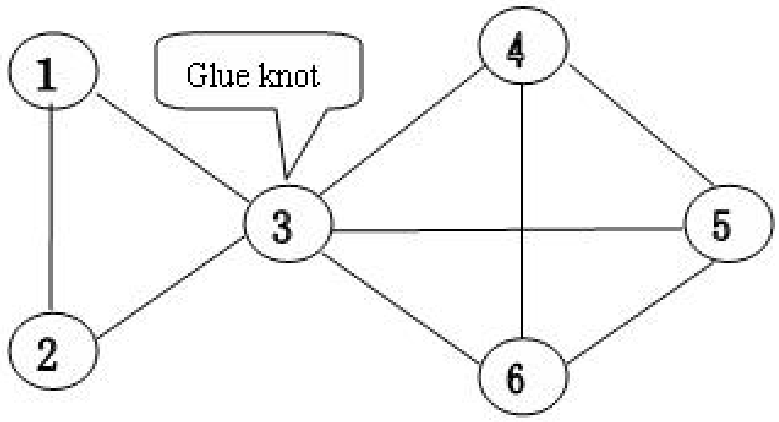

Figure 12.3: Merged graph

Write down the new transition matrix P' as

$$P' = \begin{bmatrix} .2 & .4 & .4 & 0 & 0 & 0 \\ .35 & .3 & .35 & 0 & 0 & 0 \\ .2 & .2 & \_ & .3 & .3 & .2 \\ 0 & 0 & .2 & .4 & .2 & .2 \\ 0 & 0 & .1 & .1 & .7 & .1 \\ 0 & 0 & .2 & .3 & .3 & .2 \end{bmatrix}$$

We find that the third row sums to more than one, thus we scale it by multiplying by a factor, say 0.6*. We choose the diagonal so that the row sums to 1. We get a* *final transition matrix*

$$P = \begin{bmatrix} .2 & .4 & .4 & 0 & 0 & 0 \\ .35 & .3 & .35 & 0 & 0 & 0 \\ .12 & .12 & .28 & .18 & .18 & .12 \\ 0 & 0 & .2 & .4 & .2 & .2 \\ 0 & 0 & .1 & .1 & .7 & .1 \\ 0 & 0 & .2 & .3 & .3 & .2 \end{bmatrix}$$

Check the reversibility of P using the method in Section 1.2.2.

$(P^{100})^T * P =$

$$\begin{bmatrix} 0.01213873 & 0.02427746 & 0.02427746 & 0.00000000 & 0.00000000 & 0.00000000 \\ 0.02427746 & 0.02080925 & 0.02427746 & 0.00000000 & 0.00000000 & 0.00000000 \\ 0.02427746 & 0.02427746 & 0.05664740 & 0.03641618 & 0.03641618 & 0.02427746 \\ 0.00000000 & 0.00000000 & 0.03641618 & 0.07283237 & 0.03641618 & 0.03641618 \\ 0.00000000 & 0.00000000 & 0.03641618 & 0.03641618 & 0.25491329 & 0.03641618 \\ 0.00000000 & 0.00000000 & 0.02427746 & 0.03641618 & 0.03641618 & 0.02427746 \end{bmatrix}$$

We get a symmetric matrix and conclude that P is reversible.

Now we are back to state this method and prove it.

Property 12.2.1.

A process glued from any two reversible Markov processes is reversible.

Proof. We are given two reversible Markov transition matrices $A = [a_{ij}]$ which has n states and $B = [b_{ij}]$ which has m states.

If we glue any two states of processes A and B together, say state k of A and state l of B together, we will have a $(m + n - 1)$ state space S.

Choose any path of S starting with any state and returning to that same state, eg. A path starts from state i of process A. So the Kolmogorov condition product has probability

$$a_{ii_0}a_{i_0i_1}\cdots a_{i_rk}b_{lj_0}b_{j_0j_1}\cdots b_{j_0l}a_{ki_r}a_{i_ri_{r-1}}\cdots a_{i_0i}.$$

The reversed path has the identical probability as the original path since both A and B are reversible.

Thus the Kolmogorov condition is satisfied for the glued process and thus the glued process is reversible. The scaling adjustment does not affect the reversibility as we have already seen. $\square$

Chapter 13

Summary

In this paper, we gave numerous methods (some known and many new) to create transition matrices for reversible Markov chains. We also gave operations on such matrices which will maintain the reversible nature of Markov chains. We used counting arguments to find the number of equations that are needed to check whether a Markov Chains is reversible using the Kolmogorov condition. We present a practical computer based method for checking whether or not small dimensional transition matrices correspond to reversible Markov chains. Since reversible Markov Chains appear frequently in the literature, we believe that this paper is a valuable contribution to the area.

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