

# FIRST PASSAGE PROBABILITIES

by

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# Abstract

In this paper, we consider first passage probabilities and study some of their characteristics. We first present the definition of first passage probabilities and some recurrence relationships with transition probabilities. We define two methods to compute first passage probabilities and consider some special cases. Also, we present phase-type distributions and show the similarity with first passage probabilities. Moreover, we present the inverse problem and the connection with discrete distributions.

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## CHAPTER 1

### Introduction

First passage probabilities for a discrete Markov Chain are discussed in many probability books, such as [1] and [6]. In the book, Mathematical Techniques of Applied Probability, Discrete Time Models: Basic Theory ([1]), Jeffrey Hunter defines the  $n$  step first passage time probability  $f_{ij}^{(n)}$  as follows.

DEFINITION 1.1. *Let  $\{X_n\}$  be an Markov Chain with state space  $S$ . The conditional probabilities*

$$f_{ij}^{(n)} = P(X_n = j, X_k \neq j \text{ for } k = 1, 2, \dots, n - 1 | X_0 = i) \quad (1)$$

*( $i, j \in S$ ) are called the  $n$  step first passage time probabilities and give the probability of a first passage ( $i \neq j$ ) or first return ( $i = j$ ) to state  $j$  from state  $i$  in  $n$  steps.*

For fixed  $i, j$  ( $i \neq j$ ), the first passage probabilities deal with the random variable  $N$  which is the number of steps to enter state  $j$  from  $i$  for the first time. Assume  $i \neq j$  throughout the remainder of the paper.

Hunter (1983) also presented some recurrence relationships between  $n$  step transition probabilities  $p_{ij}^{(n)}$  and  $n$  step first passage time probability  $f_{ij}^{(n)}$ . In chapter 2 of this major paper, we present a theorem from his book and we find a corollary which enables us to compute  $f_{ij}^{(n)}$ .

In chapter 3, by using the definition of  $f_{ij}^{(n)}$ , another formula can be developed for computing  $f_{ij}^{(n)}$ .

In chapter 4, we observe that for special transition matrices which have the  $j$ -th column constant, the  $n$  step first passage time probabilities  $f_{ij}^{(n)}$  follow a geometric distribution.

In chapter 5, for special transition matrices which have the  $j$ -th column with different constants with bounds, we find bounds for the mean first passage times.

In chapter 6, we comment on phase type distributions and their relation to first passage distributions.

In chapter 7 we look at the inverse problem of finding transition matrices that have prespecified first passage probabilities.

In chapter 8, we discuss the connection of first passage probability distributions with other discrete distributions.

In chapter 9, we present some situations which different transition matrices have same first passage probabilities.



## CHAPTER 2

### Computing First Passage Probabilities

Hunter(1983) presented some recurrence relationships between the  $p_{ij}^{(n)}$  and the  $f_{ij}^{(n)}$ .

THEOREM 2.1. For  $i, j \in S$ ,  $n = 1, 2, \dots$ ,

$$p_{ij}^{(n)} = \sum_{k=1}^n f_{ij}^{(k)} p_{jj}^{(n-k)} \quad (2)$$

where  $f_{ij}^{(0)} = 0$  for all  $i, j$ , and  $p_{ij}^{(0)} = 0$  for  $i \neq j$ ;  $p_{jj}^{(0)} = 1$ .

In Hlynka's course notes ([3]), he presented a proof for theorem 2.1.

PROOF. Assume  $X_0 = i$ . Let  $T_j$  denote the time of the first transition into state  $j$ . If such a transition never occurs, take  $T_j = \infty$ . By conditioning on  $T_j$ , we obtain

$$\begin{aligned} p_{ij}^{(n)} &= \sum_{k=1}^{\infty} P(X_n = j | T_j = k, X_0 = i) P(T_j = k | X_0 = i) \\ &\quad + P(X_n = j | T_j = \infty, X_0 = i) P(T_j = \infty | X_0 = i) \\ &= \sum_{k=1}^n p_{jj}^{(n-k)} f_{ij}^{(k)}. \end{aligned}$$

□

COROLLARY 2.2. For  $i, j \in S$ ,  $n = 1, 2, \dots$ ,

$$p_{ij}^{(n)} = f_{ij}^{(n)} + \sum_{k=1}^{n-1} f_{ij}^{(k)} p_{jj}^{(n-k)}. \quad (3)$$

PROOF. From theorem 2.1,

$$\begin{aligned} p_{ij}^{(n)} &= \sum_{k=1}^n f_{ij}^{(k)} p_{jj}^{(n-k)} \\ &= f_{ij}^{(n)} p_{jj}^{(0)} + \sum_{k=1}^{n-1} f_{ij}^{(k)} p_{jj}^{(n-k)} \\ &= f_{ij}^{(n)} + \sum_{k=1}^{n-1} f_{ij}^{(k)} p_{jj}^{(n-k)}. \end{aligned}$$

( since  $p_{jj}^{(0)} = 1$  )

□

COROLLARY 2.3. From corollary 2.2,

$$f_{ij}^{(n)} = p_{ij}^{(n)} - \sum_{k=1}^{n-1} f_{ij}^{(k)} p_{jj}^{(n-k)}. \quad (4)$$

Corollary 2.3 gives a general recursive formula for computing  $f_{ij}^{(n)}$ .

## CHAPTER 3

### Another Computational Method

By definition,  $f_{ij}^{(n)}$  is the probability that the system enters state  $j$  for the first time at step  $n$  from state  $i$ . That means it never enters state  $j$  for the first  $n - 1$  steps, and arrives to state  $j$  at the last step. By using this idea, we create another formula for  $f_{ij}^{(n)}$ . This formula is likely known, but we could not find it in the literature. The closely related phase type distributions use essentially this formula.

**THEOREM 3.1.** *Let  $P = [p_{ij}]$  denote the transition matrix for a Markov chain, where  $p_{ij} = P(X_{n+1} = j | X_n = i)$ . Let  $P'$  be the matrix obtained by replacing  $j$ -th column of  $P$  by the zero vector. Then*

$$f_{ij}^{(n)} = p_{i \cdot}^{\prime(n-1)} \cdot p_{\cdot j} \quad (5)$$

where  $p_{i \cdot}^{\prime(n-1)}$  is the  $i$ -th row of the of  $(P')^{n-1}$ , and  $p_{\cdot j}$  is the  $j$ -th column of transition matrix  $P$ .

We illustrate the result using an examples of a  $3 \times 3$  numeric matrices. The results from both procedures are the same.

Example: Given  $P = \begin{bmatrix} .6 & .3 & .1 \\ .6 & .2 & .2 \\ .3 & .3 & .4 \end{bmatrix}$ , find  $f_{13}^{(n)}$ .

$$P' = \begin{bmatrix} 0.6 & 0.3 & 0 \\ 0.6 & 0.2 & 0 \\ 0.3 & 0.3 & 0 \end{bmatrix}.$$

$$f_{13}^{(2)} = 0.6 \times 0.1 + 0.3 \times 0.2 = 0.12.$$

$$f_{13}^{(2)} = p'_{1.} \cdot p_{.3} = 0.12.$$

$$\begin{aligned} f_{13}^{(3)} &= p_{13}^{(3)} - f_{13}^{(1)} p_{33}^{(2)} - f_{13}^{(2)} p_{33}^{(1)} \\ &= 0.175 - 0.1 \times 0.25 - 0.12 \times 0.4 \\ &= 0.102. \end{aligned}$$

$$f_{13}^{(3)} = p'_{1.}^{(2)} \cdot p_{.3} = 0.102.$$

$$\begin{aligned} f_{13}^{(4)} &= p_{13}^{(4)} - f_{13}^{(1)} p_{33}^{(3)} - f_{13}^{(2)} p_{33}^{(2)} - f_{13}^{(3)} p_{33}^{(1)} \\ &= 0.1798 - 0.1 \times 0.202 - 0.12 \times 0.25 - 0.102 \times 0.4 \\ &= 0.0888. \end{aligned}$$

$$f_{13}^{(4)} = p'_{1.}^{(3)} \cdot p_{.3} = 0.0888.$$

$$\begin{aligned}
f_{13}^{(5)} &= p_{13}^{(5)} - f_{13}^{(1)} p_{33}^{(4)} - f_{13}^{(2)} p_{33}^{(3)} - f_{13}^{(3)} p_{33}^{(2)} - f_{13}^{(4)} p_{33}^{(1)} \\
&= 0.18121 - 0.1 \times 0.1879 - 0.12 \times 0.202 - 0.102 \times 0.25 - 0.0888 \times 0.4 \\
&= 0.07716.
\end{aligned}$$

$$f_{13}^{(5)} = p_{1.}^{(4)} \cdot p_{.3} = 0.07716.$$

$$\begin{aligned}
f_{13}^{(6)} &= p_{13}^{(6)} - f_{13}^{(1)} p_{33}^{(5)} - f_{13}^{(2)} p_{33}^{(4)} - f_{13}^{(3)} p_{33}^{(3)} - f_{13}^{(4)} p_{33}^{(2)} - f_{13}^{(5)} p_{33}^{(1)} \\
&= 0.181636 - 0.1 \times 0.18364 - 0.12 \times 0.1879 - 0.102 \times 0.202 - 0.0888 \times 0.25 \\
&\quad - 0.07716 \times 0.4 \\
&= 0.067056.
\end{aligned}$$

$$f_{13}^{(6)} = p_{1.}^{(5)} \cdot p_{.3} = 0.067056.$$

$$\begin{aligned}
f_{13}^{(7)} &= p_{13}^{(7)} - f_{13}^{(1)} p_{33}^{(6)} - f_{13}^{(2)} p_{33}^{(5)} - f_{13}^{(3)} p_{33}^{(4)} - f_{13}^{(4)} p_{33}^{(3)} - f_{13}^{(5)} p_{33}^{(2)} - f_{13}^{(6)} p_{33}^{(1)} \\
&= 0.1817635 - 0.1 \times 0.182365 - 0.12 \times 0.18364 - 0.102 \times 0.1879 \\
&\quad - 0.0888 \times 0.202 - 0.07716 \times 0.25 - 0.067056 \times 0.4 \\
&= 0.0582744.
\end{aligned}$$

$$f_{13}^{(7)} = p_{1.}^{(6)} \cdot p_{.3} = 0.0582744.$$

$$\begin{aligned}
f_{13}^{(8)} &= p_{13}^{(8)} - f_{13}^{(1)} p_{33}^{(7)} - f_{13}^{(2)} p_{33}^{(6)} - f_{13}^{(3)} p_{33}^{(5)} - f_{13}^{(4)} p_{33}^{(4)} - f_{13}^{(5)} p_{33}^{(3)} - f_{13}^{(6)} p_{33}^{(2)} - f_{13}^{(7)} p_{33}^{(1)} \\
&= 0.1818018 - 0.1 \times 0.1819822 - 0.12 \times 0.182365 - 0.102 \times 0.18364 \\
&\quad - 0.0888 \times 0.1879 - 0.07716 \times 0.202 - 0.067056 \times 0.25 - 0.0582744 \times 0.4 \\
&= 0.0506429.
\end{aligned}$$

$$f_{13}^{(8)} = p_{1.}^{(7)} \cdot p_{.3} = 0.0506429.$$

## CHAPTER 4

### Connection with the Geometric Distribution

For some special cases, the transition matrices have the  $j$ -th column with the same constant  $\alpha$ . Then their  $n$  step first passage probabilities follow the geometric distribution.

**THEOREM 4.1.** *If the transition matrix for a Markov Chain has its  $j$ -th column with the same constant  $\alpha$  (except perhaps in row  $j$ ), say*

$$P = \begin{bmatrix} \cdots & \alpha & \cdots \\ \cdots & \alpha & \cdots \\ \cdots & \vdots & \cdots \\ \cdots & \alpha & \cdots \end{bmatrix}$$

*then its  $n$  step first passage probabilities from  $i$  to  $j$  (for fixed  $i$  and  $j$ ) form a geometric distribution,  $f_{ij}^{(n)} \sim \text{Geometric}(\alpha)$ .*

**PROOF.** The sum of any row of a transition matrix equals 1. Thus for  $v = 2, 3, \dots$ ,

$$P^v = P^{v-1} \times P.$$

So

$$\begin{aligned} p_{ij}^{(v)} &= (i\text{-th row of } P^{v-1}) \bullet (j\text{-th column of } P) \\ &= (\text{sum of entries of row } i \text{ of } P^{v-1}) \times \alpha \end{aligned}$$

$$= (1)\alpha$$

$$= \alpha.$$

Hence

$$\begin{aligned} f_{ij}^{(n)} &= p_{ij}^{(n)} - \sum_{v=1}^{n-1} f_{ij}^{(v)} p_{jj}^{(n-v)} \\ &= \alpha - \alpha \sum_{v=1}^{n-1} f_{ij}^{(v)} \\ &= \alpha - \alpha(f_{ij}^{(1)} + f_{ij}^{(2)} + f_{ij}^{(3)} + f_{ij}^{(4)} + \cdots + f_{ij}^{(n-1)}). \end{aligned}$$

$$f_{ij}^{(1)} = \alpha,$$

$$f_{ij}^{(2)} = \alpha - \alpha f_{ij}^{(1)} = \alpha(1 - \alpha),$$

$$f_{ij}^{(3)} = \alpha - \alpha(f_{ij}^{(1)} + f_{ij}^{(2)}) = \alpha(1 - \alpha)^2,$$

$$f_{ij}^{(4)} = \alpha - \alpha(f_{ij}^{(1)} + f_{ij}^{(2)} + f_{ij}^{(3)}) = \alpha(1 - \alpha)^3,$$

$\vdots$

$$f_{ij}^{(n-1)} = \alpha(1 - \alpha)^{n-2}.$$

$$\begin{aligned} \therefore f_{ij}^{(n)} &= \alpha - \alpha\{\alpha + \alpha(1 - \alpha) + \alpha(1 - \alpha)^2 + \cdots + \alpha(1 - \alpha)^{n-2}\} \\ &= \alpha - \alpha^2\{1 + (1 - \alpha) + (1 - \alpha)^2 + \cdots + (1 - \alpha)^{n-2}\} \\ &= \alpha - \alpha^2 \times \frac{1 - (1 - \alpha)^{n-1}}{1 - (1 - \alpha)} \\ &= \alpha - \alpha \times \{1 - (1 - \alpha)^{n-1}\} \end{aligned}$$



$$= \alpha\{1 - 1 + (1 - \alpha)^{n-1}\}$$

$$= \alpha(1 - \alpha)^{n-1}.$$

$\therefore f_{ij}^{(n)} \sim \text{Geometric}(\alpha).$

□

Again, we illustrate the result using a matrix example. By comparing with theorem 3.1, the results from both methods are the same.

Example: Given  $P = \begin{bmatrix} 0.2 & 0.1 & 0.7 \\ 0.3 & 0.1 & 0.6 \\ 0.5 & 0.1 & 0.4 \end{bmatrix}$ , find  $f_{12}^{(n)}$  using both methods

$f_{ij}^{(n)} = p_i'^{(n-1)} \cdot p_{.j}$  and  $f_{ij}^{(n)} = \alpha(1 - \alpha)^{(n-1)}$ .

$$P' = \begin{bmatrix} 0.2 & 0 & 0.7 \\ 0.3 & 0 & 0.6 \\ 0.5 & 0 & 0.4 \end{bmatrix}.$$

$$f_{12}^{(2)} = 0.2 \times 0.1 + 0.7 \times 0.1 = 0.09.$$

$$f_{12}^{(2)} = 0.1 \times (1 - 0.1)^{2-1} = 0.09.$$

$$f_{12}^{(3)} = p_1'^{(2)} \cdot p_{.2} = 0.081.$$

$$f_{12}^{(3)} = 0.1(1 - 0.1)^{3-1} = 0.081.$$

$$f_{12}^{(6)} = p_1'^{(5)} \cdot p_{.2} = 0.059049.$$

$$f_{12}^{(6)} = 0.1(1 - 0.1)^{6-1} = 0.059049.$$

$$f_{12}^{(10)} = p_{1.}^{(9)} \cdot p_{.2} = 0.03874205.$$

$$f_{12}^{(10)} = 0.1 \times 0.9^9 = 0.03874205.$$

$$f_{12}^{(20)} = p_{1.}^{(19)} \cdot p_{.2} = 0.01350852.$$

$$f_{12}^{(20)} = 0.1 \times 0.9^{19} = 0.01350852.$$

## CHAPTER 5

### Bounds of the mean first passage times

Suppose that the  $j$ -th column of the transition matrix has entries  $\alpha_1, \alpha_2, \dots, \alpha_m$  with  $\beta \leq \alpha_i \leq \gamma$ . Assume  $X_0 = i$ . Define  $T_j = \{ \min n | X_n = j \}$ .  $T_j$  is called a first passage time. We find bounds for the mean first passage times.

**THEOREM 5.1.** *Suppose the transition matrix for a Markov Chain has  $j$ -th column with entries  $\alpha_1, \alpha_2, \dots, \alpha_m$  with  $\beta \leq \alpha_i \leq \gamma$ ,*

$$P = \begin{bmatrix} \cdots & \alpha_1 & \cdots \\ \cdots & \alpha_2 & \cdots \\ \cdots & \vdots & \cdots \\ \cdots & \alpha_m & \cdots \end{bmatrix}.$$

*Let  $P^{**}$  and  $P^*$  be new matrices obtained by replacing all entries of  $j$ -th column in  $P$  by  $\beta$  and  $\gamma$ , respectively; and adjusting the remaining entries of each row proportionally, so that the row sums are 1.*

$$P^{**} = \begin{bmatrix} \cdots & \beta & \cdots \\ \cdots & \beta & \cdots \\ \cdots & \vdots & \cdots \\ \cdots & \beta & \cdots \end{bmatrix}$$

$$P^* = \begin{bmatrix} \cdots & \gamma & \cdots \\ \cdots & \gamma & \cdots \\ \cdots & \vdots & \cdots \\ \cdots & \gamma & \cdots \end{bmatrix}$$

Let  $T_j$  be the first passage time with transition matrix  $P$ ;  $T_j^{**}$  and  $T_j^*$  be the first passage times with transition matrices  $P^{**}$  and  $P^*$ , respectively. Then

$$E(T_j^*) \leq E(T_j) \leq E(T_j^{**}) \quad (6)$$

PROOF. Recall that for a discrete random variable  $X$  on  $S = 0, 1, \dots$ , we know  $E(X) = \sum_{n=0}^{\infty} P(X > n)$ . Assume  $X_0 = i$ . Thus  $E(T_j) = \sum_{n=0}^{\infty} P_i(T_j > n)$ .

$$\begin{aligned} P_i(T_j > n) &= P(X_1 \neq j, \dots, X_n \neq j) \\ &= \sum_{k:k \neq j} P(X_1 \neq j, \dots, X_{n-2} \neq j, X_{n-1} = k, X_n \neq j) \\ &= \sum_{k:k \neq j} P(X_1 \neq j, \dots, X_{n-2} \neq j, X_{n-1} = k) P(X_n \neq j | X_{n-1} = k) \\ &= \sum_{k:k \neq j} P(X_1 \neq j, \dots, X_{n-2} \neq j, X_{n-1} = k) (1 - p_{kj}) \\ &\leq \sum_{k:k \neq j} P(X_1 \neq j, \dots, X_{n-2} \neq j, X_{n-1} = k) (1 - \beta) \\ &= P(X_1 \neq j, \dots, X_{n-2} \neq j, X_{n-1} \neq j) (1 - \beta) \\ &\dots \\ &= (1 - \beta)^n. \end{aligned}$$

That is,  $P_i(T_j > n) \leq (1 - \beta)^n$ .

Similarly,  $(1 - \gamma)^n \leq P_i(T_j > n)$ .

So,  $(1 - \gamma)^n \leq P_i(T_j > n) \leq (1 - \beta)^n$ .

Hence,  $\sum_{n=0}^{\infty} (1 - \gamma)^n \leq \sum_{n=0}^{\infty} P_i(T_j > n) \leq \sum_{n=0}^{\infty} (1 - \beta)^n$ .

Therefore,  $E(T_j^*) \leq E(T_j) \leq E(T_j^{**})$ . □

Note that if  $\beta = \gamma = \alpha$  in the above result, then  $P_i(T_j > n) = (1 - \beta)^n = (1 - \gamma)^n$ .

So,  $T_j \sim \text{Geometric}(\beta)$ .

In Hunter's book ([1]), there is a theorem for the mean first passage times.

**THEOREM 5.2.** *Let  $P = [p_{ij}]$  be the transition matrix of an irreducible Markov Chain. Then, for all  $i, j \in S$ ,*

$$\mu_{ij} = 1 + \sum_{k \neq j} p_{ik} \mu_{kj} \tag{7}$$

where  $\mu_{ij} = E(T_j)$ .

From theorem 5.2, we develop a corollary which is more useful for computation.

COROLLARY 5.3. Let  $\underline{E}_j = \begin{bmatrix} \mu_{1j} \\ \vdots \\ \mu_{jj} \\ \vdots \\ \mu_{mj} \end{bmatrix}$ , where  $\mu_{ij} = E(T_j)$ , for  $i = 1, \dots, m$ .

Then

$$\underline{E}_j = (I - P')^{-1}e. \quad (8)$$

where  $e$  is a column vector of 1's.

PROOF. By theorem 5.2,

$$\underline{E}_j = \begin{bmatrix} \mu_{1j} \\ \vdots \\ \mu_{jj} \\ \vdots \\ \mu_{mj} \end{bmatrix} = e + P' \underline{E}_j \quad (9)$$

$$\Rightarrow \underline{E}_j = e + P' \underline{E}_j$$

$$\Rightarrow \underline{E}_j - P' \underline{E}_j = e$$

$$\Rightarrow (I - P') \underline{E}_j = e$$

$$\Rightarrow \underline{E}_j = (I - P')^{-1}e$$

□

We illustrate the theorem 4.1 and corollary 5.3 using a matrix example. The results show that the mean first passage times are bounded.

Example:

$$P = \begin{bmatrix} 0.6 & 0.3 & 0.1 \\ 0.6 & 0.2 & 0.2 \\ 0.3 & 0.3 & 0.4 \end{bmatrix}.$$

$$P' = \begin{bmatrix} 0.6 & 0 & 0.1 \\ 0.6 & 0 & 0.2 \\ 0.3 & 0 & 0.4 \end{bmatrix}.$$

$$E_2 = \begin{bmatrix} \mu_{12} \\ \mu_{22} \\ \mu_{32} \end{bmatrix} = (I - P')^{-1}e = \begin{bmatrix} 3.333 \\ 3.6667 \\ 3.333 \end{bmatrix}.$$

$$\beta = 0.2$$

$$\implies P^{**} = \begin{bmatrix} \frac{6}{7} \times 0.8 & 0.2 & \frac{1}{7} \times 0.8 \\ 0.6 & 0.2 & 0.2 \\ \frac{3}{7} \times 0.8 & 0.2 & \frac{4}{7} \times 0.8 \end{bmatrix} = \begin{bmatrix} \frac{4.8}{7} & 0.2 & \frac{0.8}{7} \\ 0.6 & 0.2 & 0.2 \\ \frac{2.4}{7} & 0.2 & \frac{3.2}{7} \end{bmatrix}$$

$$\implies T_2^{**} \sim \text{Geometric}(0.2)$$



$$\implies E(T_2^{**}) = \frac{1-0.2}{0.2} = 4.$$

$$\gamma = 0.3$$

$$\implies P^* = \begin{bmatrix} 0.6 & 0.3 & 0.1 \\ \frac{6}{8} \times 0.7 & 0.3 & \frac{2}{8} \times 0.7 \\ 0.3 & 0.3 & 0.4 \end{bmatrix} = \begin{bmatrix} 0.6 & 0.3 & 0.1 \\ \frac{4.3}{8} & 0.3 & \frac{1.4}{8} \\ 0.3 & 0.3 & 0.4 \end{bmatrix}$$

$$\implies T_2^* \sim \text{Geometric}(0.3)$$

$$\implies E(T_2^*) = \frac{1-0.3}{0.3} = \frac{7}{3}.$$

$$\therefore E_2^* \leq E_2 \leq E_2^{**}.$$

## CHAPTER 6

### Connection with Phase-Type Distributions

As introduced by Neuts([7]) and discussed in Latouche and Ramaswami ([4]) (p. 47), phase-type distributions are defined as follows.

Phase-Type Distributions: Consider a finite Markov chain with a single absorbing state (the first state) and  $m$  other states. Partition the probability transition matrix as

$$P = \begin{bmatrix} 1 & 0 \\ t & T \end{bmatrix}$$

where  $T$  is a matrix of order  $m$  and  $t$  is a column vector. Let the initial probability row vector be  $\tau$ . The probabilities of reaching the absorbing state at time  $n$  are called phase-type probabilities and are the components of  $\tau T^{n-1}t$ .

The first passage probabilities and phase-type probabilities seem to be almost the same, but the phase type distribution requires an initial probability vector. This initial probability vector allows phase type distributions to represent any probability distribution with finite support  $\{p_i\}$ , ( $i = 1, \dots, n$ ) as a phase type distribution by simply selecting  $\tau = (p_1, \dots, p_n)$ , and choosing the matrix  $T$  with entries  $T_{i,i-1} = 1$ . Without the initial probability vector, (or with an initial probability vector that begins in a particular state with probability 1), it is unclear as to whether an arbitrary probability distribution with positive integer finite support could be represented. This question is answered in the next section.

## CHAPTER 7

### The Inverse Problem

In this chapter, we present a method to find transition matrices such that the first passage probabilities form a prespecified discrete finite probability mass function.

Mandelbaum, Hlynka and Brill ([5]) introduced nonhomogeneous probability distributions. They found that nonhomogeneous geometric distributions could cover all discrete distributions with finite positive integer support. We use this idea in the following theorem.

**THEOREM 7.1.** *Suppose we have prespecified probabilities  $a_n$ ,  $n = 1, 2, \dots, k$ ; where  $\sum_{n=1}^k a_n = 1$ . Then one matrix  $P$  (not unique) with first passage probabilities*

*$f_{1,k+1}^{(n)} = a_n$  is given by  $P = [p_{ij}]$  where  $P$  is a  $(k+1) \times (k+1)$  matrix with*

$$p_{1,k+1} = a_1, \quad p_{12} = 1 - a_1,$$

$$p_{i,k+1} = \frac{a_i}{1 - a_1 - a_2 - \dots - a_{i-1}}, \quad \text{for } i = 2, \dots, k-1,$$

$$p_{i,i+1} = \frac{1 - a_1 - \dots - a_i}{1 - a_1 - a_2 - \dots - a_{i-1}}, \quad \text{for } i = 2, \dots, k-1,$$

$$p_{k,k+1} = 1,$$

$$p_{ij} = 0 \quad \text{for } i = 1, \dots, k; j \neq i+1, k+1,$$

*and  $p_{k+1,j}$  is arbitrary subject to*

$$0 \leq p_{k+1,j} \leq 1, \quad \sum_{j=1}^{k+1} p_{k+1,j} = 1.$$

PROOF. In order to move from state 1 to state  $k + 1$  for the first time in exactly 1 step, we must move from state 1 to state  $k + 1$  on the first step. Thus  $f_{1,k+1}^{(1)} = p_{1,k+1} = a_1$ . We then choose  $p_{1,2} = 1 - a_1$ .

Note that from state 1, we can only move to state 2 or state  $k + 1$ . In order to move from state 1 to state  $k + 1$  for the first time in exactly 2 steps, we must move from state 1 to state 2 on the first step and from state 2 to state  $k + 1$  on the second step.

Thus

$$f_{1,k+1}^{(2)} = p_{12}p_{2,k+1} = a_2, \text{ so } p_{2,k+1} = \frac{a_2}{p_{12}} = \frac{a_2}{1-a_1}. \text{ We then choose } p_{23} = 1 - \frac{a_2}{1-a_1} = \frac{1-a_1-a_2}{1-a_1}.$$

Similarly, we find

$$p_{i,k+1} = \frac{a_i}{1-a_1-a_2-\dots-a_{i-1}}, \text{ for } i = 2, \dots, k-1. \text{ We choose}$$

$$p_{i,i+1} = \frac{1-a_1-\dots-a_i}{1-a_1-a_2-\dots-a_{i-1}}, \text{ for } i = 2, \dots, k-1.$$

After state  $k$ , we are forced to move to state  $k + 1$  so  $p_{k,k+1} = 1$ .

Then,  $f_{1,k+1}^{(n)} = a_n$  for  $n = 1, \dots, k$ . □

Example 1: Let  $Y = X + 1$ , where  $X \sim \text{Binomial}(3, 0.5)$ . Then

$$f(x) = 0.25 \text{ for } x = 1,$$

$$f(x) = 0.5 \text{ for } x = 2,$$

$$f(x) = 0.25 \text{ for } x = 3.$$

Then  $a_1 = 0.25, a_2 = 0.5, a_3 = 0.25$ .

Let  $k = 3$ , then  $k + 1 = 4$ . Take

$$p_{14} = 0.25, \text{ and } p_{12} = 1 - 0.25 = 0.75;$$

$$p_{24} = \frac{a_2}{1-a_1} = \frac{0.5}{1-0.25} = \frac{2}{3};$$

$$p_{23} = 1 - \frac{2}{3} = \frac{1}{3};$$

$$p_{34} = 1.$$

The last row of  $P$  is arbitrary. Take

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

Then

$$f_{14}^{(1)} = 0.25;$$

$$f_{14}^{(2)} = 0.5;$$

$$f_{14}^{(3)} = 0.25;$$

$$f_{14}^{(n)} = 0 \text{ for } n = 4, 5, \dots.$$

Example 2: Given  $f_{17}^{(n)} = 0$  for  $n = 1, 2, 3$ ,  $f_{17}^{(4)} = 0.3$ ,  $f_{17}^{(5)} = 0.5$ ,  $f_{17}^{(6)} = 0.2$ , find a matrix  $P$  which satisfies these conditions.

SOLUTION:

Since  $k = 6$ , then  $k + 1 = 7$  and the matrix  $P$  is  $7 \times 7$ .

Take  $p_{i,i+1} = 1$  for  $k = 1, 2, 3$ ,  $p_{k,k+1} = 1$ .

By our theorem, we select

$$p_{47} = 0.3, p_{45} = 1 - 0.3 = 0.7;$$

$$p_{57} = \frac{0.5}{1-0.3} = \frac{5}{7}, p_{56} = 1 - \frac{5}{7} = \frac{2}{7}.$$

$$\text{Hence } P = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.7 & 0 & 0.3 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{7} & \frac{5}{7} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ * & * & * & * & * & * & * \end{bmatrix} \text{ where the last row of } P \text{ is arbitrary.}$$

We can use this approach to get a transition matrix for any given distribution with discrete finite support of positive integers (such as a zero truncated binomial distribution).

However, one difficulty with this approach is that the size of the matrix needed can be quite large.

For a distribution with infinite support on the positive integers such as a zero truncated Poisson distribution, we can approximate the first passage probabilities by truncating the distribution after some large number of steps but that means that the transition matrix  $P$  will be large as well.

## CHAPTER 8

### Connection with Discrete Distributions

We know that the phase-type distribution can generalize all discrete distributions with finite support (see [4]). As we discovered in chapter 6, the first passage probability distributions and phase-type distributions are almost identical. Therefore, first passage probability distributions include all discrete distributions with finite support.

From theorem 4.1, the first passage probabilities  $f_{ij}^{(n)}$  ( $i \neq j$ , for fixed  $i, j$ ) of a transition matrix which has the same constant in the  $j$ -th column follow a geometric distribution.

Then we can write a  $2 \times 2$  case as

$$P = \begin{bmatrix} 1-p & p \\ * & * \end{bmatrix}$$

$$\Rightarrow f_{12}^{(n)} = (1-p)^{n-1}p \text{ for } n = 1, 2, \dots$$

By using this idea, we can obtain matrices which have first passage probabilities for negative binomial random variables since negative binomial random variables are the sum of geometric random variables. For example consider the following  $4 \times 4$  matrix.

$$P = \begin{bmatrix} 1-p & p & 0 & 0 \\ 0 & 1-p & p & 0 \\ 0 & 0 & 1-p & p \\ * & * & * & * \end{bmatrix}$$

$$\Rightarrow f_{14}^{(n)} = \binom{n-1}{2} p^3 (1-p)^{n-3} \text{ for } n = 3, 4, \dots$$

$\Rightarrow$  The first passage probability follows a negative binomial with  $k = 3$ .

In general, take  $P$  to be a  $(k+1) \times (k+1)$  matrix with

$$p_{ii} = 1-p \text{ for } i = 1, \dots, k,$$

$$p_{i,i+1} = p \text{ for } i = 1, \dots, k,$$

$$p_{ij} = 0 \text{ for } i = 1, \dots, k; j \neq i, i+1,$$

$$p_{k+1,j} \text{ arbitrary such that } \sum_{j=1}^{k+1} p_{k+1,j} = 1, 0 \leq p_{k+1,j} \leq 1$$

$$\Rightarrow f(n) = \binom{n-1}{k-1} p^k (1-p)^{n-k} \text{ for } n = k, k+1, \dots$$

$\Rightarrow$  The first passage probability follows negative binomial distribution with parameters  $k$  and  $p$ .

Also, we can develop a matrix for a shifted geometric distribution.

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1-p & p \\ * & * & * & * \end{bmatrix}$$

$$\Rightarrow f_{14}^{(n)} = (1-p)^{n-3} p \text{ for } n = 3, 4, \dots$$



$\Rightarrow$  The first passage probability follows a shifted geometric distribution.

The above results suggest that a geometric distribution would allow considerable flexibility in finding transition matrices to correspond prespecified distributions.

Moreover, the first passage probabilities don't just follow a geometric distribution. They may have some unusual patterns.

Example 1: Given  $P = \begin{bmatrix} 0 & 1 & 0 \\ 0.5 & 0 & 0.5 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}$ ,

we get the first passage probabilities from state 1 to state 3 as follows.

For  $n = 1, 3, 5, \dots$ ,  $f_{13}^{(n)} = 0$ ;

For  $n = 2, 4, 6, \dots$ ,  $f_{13}^{(n)} = (0.5)^{\frac{n}{2}}$ .

By plotting these first passage probabilities, we get a graph of the type in Figure 8.1.

Example 2: Given  $P = \begin{bmatrix} 0 & 0.9 & 0.1 \\ 0.5 & 0 & 0.5 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}$ ,

we get the first passage probabilities from state 1 to state 3 as follows.

For  $n = 1, 3, 5, \dots$ ,  $f_{13}^{(n)} = \frac{(0.45)^{\frac{n}{2}}}{10}$ ;

For  $n = 2, 4, 6, \dots$ ,  $f_{13}^{(n)} = (0.45)^{\frac{n}{2}}$ .

By plotting these first passage probabilities, we get a graph as in Figure 8.2.

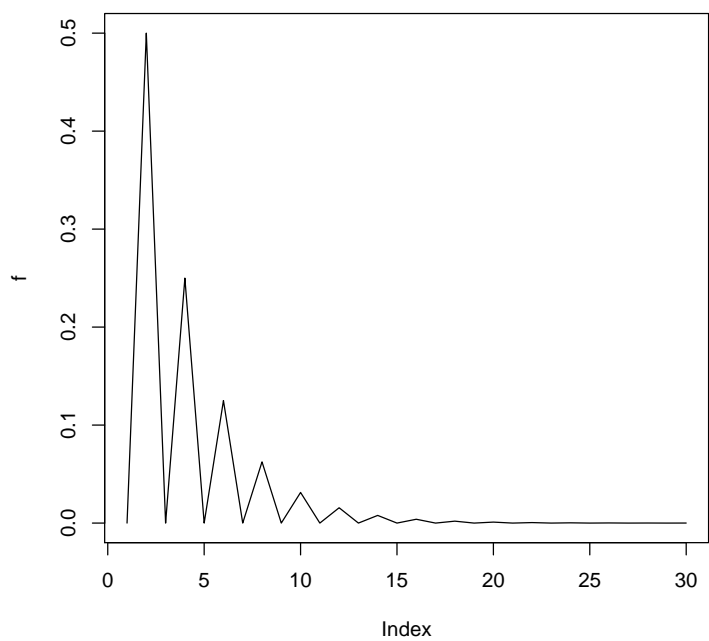


FIGURE 8.1. Unusual Pattern of First Passage Probabilities (1)

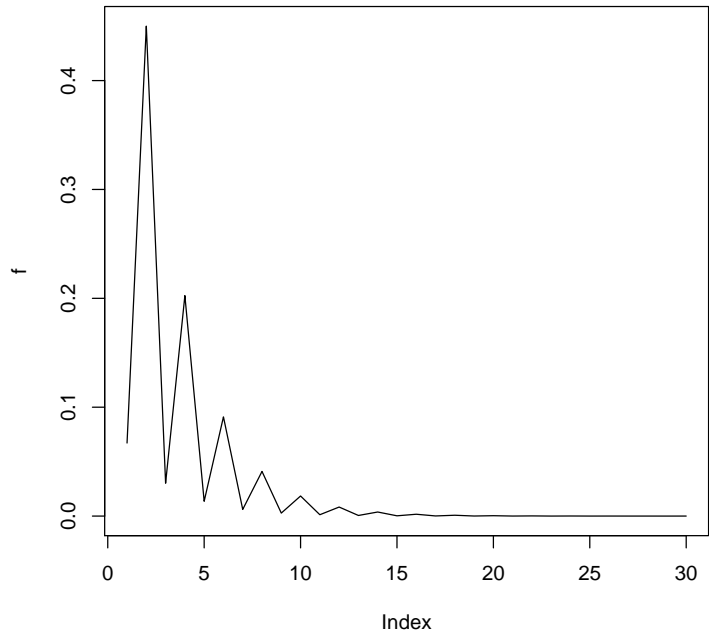


FIGURE 8.2. Unusual Pattern of First Passage Probabilities (2)

## CHAPTER 9

### Different transition matrices with same first passage probabilities

We know that under some circumstances, we can have  $P_1, P_2$  which have the same size  $(k + 1) \times (k + 1)$  but different entries, yet

$$f_{1,k+1}^{(n)} = F_{1,k+1}^{(n)}$$

where  $f$  is the first passage probabilities corresponding to  $P_1$ , and  $F$  is the first passage probabilities corresponding to  $P_2$ .

One situation is the geometric case where columns  $k + 1$  of two transition matrices are same.

For example:

$$P_1 = \begin{bmatrix} 0.6 & 0.1 & 0.3 \\ 0.5 & 0.2 & 0.3 \\ * & * & * \end{bmatrix}$$

$$P_2 = \begin{bmatrix} 0.4 & 0.3 & 0.3 \\ 0.3 & 0.4 & 0.3 \\ * & * & * \end{bmatrix}$$

The first passage probabilities from state 1 to state 3 are same corresponding to transition matrices  $P_1$  and  $P_2$ .

Another situation is to make a change in labeling on states other than state 1 or  $k + 1$ .

For example:

$$P_1 = \begin{bmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \\ * & * & * & * \end{bmatrix}$$

$$P_2 = \begin{bmatrix} a & c & b & d \\ i & k & j & l \\ e & g & f & h \\ * & * & * & * \end{bmatrix}$$

have the same first passage probabilities from state 1 to state 4 since we have performed a label change  $2 \leftrightarrow 3$  for states 2 and 3.

There are examples other than those of the two types mentioned which will give the same first passage probabilities. One such example follows.

Example:

$$P_1 = \begin{bmatrix} 0 & 0.4 & 0.288 & 0.112 & 0.2 \\ 0 & 0 & 0.8 & 0 & 0.2 \\ 0 & 0 & 0 & 0.625 & 0.375 \\ 0 & 0 & 0 & 0 & 1 \\ * & * & * & * & * \end{bmatrix}$$

$$P_2 = \begin{bmatrix} 0 & 0.5 & 0.2625 & 0.0375 & 0.2 \\ 0 & 0 & 0.7 & 0 & 0.3 \\ 0 & 0 & 0 & \frac{4}{7} & \frac{3}{7} \\ 0 & 0 & 0 & 0 & 1 \\ * & * & * & * & * \end{bmatrix}$$

These two different matrices have the same first passage probabilities from state 1 to state 5 with  $f_{15}^{(1)} = 0.2$ ,  $f_{15}^{(2)} = 0.3$ ,  $f_{15}^{(3)} = 0.3$ ,  $f_{15}^{(4)} = 0.2$ .

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