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## TRIANGULAR STOCHASTIC MATRICES GENERATED BY INFINITESIMAL ELEMENTS

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Abstract. We show that each element in the semigroup  $S_n$  of all  $n \times n$  non-singular upper (or lower) triangular stochastic matrices is generated by the infinitesimal elements of  $S_n$ , which form a cone consisting of all  $n \times n$  upper (or lower) triangular intensity matrices.

MSC 2000: 22E99

#### 1. INTRODUCTION

Let G be a Lie group, let L(G) be its Lie algebra, and let exp:  $L(G) \to G$  denote the exponential mapping. Let  $gl(n, \mathbb{R})$  denote the set of all real  $n \times n$  matrices and  $GL(n, \mathbb{R})$  the general linear group of degree n over  $\mathbb{R}$ . Here  $\mathbb{R}$  denotes the set of all real numbers and hereafter we shall use this notation. For  $G = GL(n, \mathbb{R})$  and  $L(G) = gl(n, \mathbb{R})$ , it is well known that the exponential map exp:  $gl(n, \mathbb{R}) \to GL(n, \mathbb{R})$ is defined by  $exp(tX) = I + tX + \frac{1}{2!}(tX)^2 + \ldots$  for  $X \in gl(n, \mathbb{R})$ .

Let  $S_n$  be a subsemigroup of  $\operatorname{GL}(n, \mathbb{R})$  and let X(t) be a differentiable matrix function of the real parameter t in an interval  $0 \leq t \leq t_0$  such that  $X(t) \in S_n$  for each t and X(0) = I. We call the matrix  $\left(\frac{\mathrm{d}X(t)}{\mathrm{d}t}\right)|_{t=0}$  an *infinitesimal element* of  $S_n$ and denote the totality of all infinitesimal elements of  $S_n$  by  $\mathscr{D}(S_n)$ . Let A(t) be a sectionwise continuous function of t ( $0 \leq t \leq t_0$ ) such that  $A(t) \in \mathscr{D}(S_n)$  for each t. It is standard that the differential equation

$$\frac{\mathrm{d}X(t)}{\mathrm{d}t} = A(t)X(t); \quad X(0) = I$$

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has a unique continuous solution and  $X(t_0) \in S_n$ . This  $X(t_0)$  in  $S_n$  is called generated by the infinitesimal elements A(t)  $(0 \leq t \leq t_0)$ .

Loewner [3] showed that each element in the semigroup of all  $n \times n$  non-singular totally positive matrices is generated by the infinitesimal elements of the semigroup, which form a set of all  $n \times n$  Jacobi matrices with non-negative off-diagonal elements. In general, a semigroup is not completely recreated from its infinitesimal elements, even if the semigroup is connected, and it is quite difficult to compute a semigroup generated by its infinitesimal elements.

In Section 2, we show that the infinitesimal elements of the semigroup of all  $n \times n$ non-singular upper (or lower) triangular stochastic matrices are  $n \times n$  upper (or lower) triangular intensity matrices. Finally, in Section 3, we show that each element in the semigroup  $S_n$  of all  $n \times n$  non-singular upper (or lower) triangular stochastic matrices is generated by the infinitesimal elements of  $S_n$ , which form a cone consisting of all  $n \times n$  upper (or lower) triangular intensity matrices.

#### 2. Infinitesimal elements of triangular stochastic matrices

**Definition.** A matrix  $A = ||a_{ij}||$  (i = 1, 2, ..., m; j = 1, 2, ..., n) over  $\mathbb{R}$  is called a stochastic matrix if  $a_{ij} \ge 0$  and  $\sum_{j=1}^{n} a_{ij} = 1$  for i = 1, 2, ..., m. A matrix  $B = ||b_{kl}||$ (k = 1, 2, ..., m; l = 1, 2, ..., n) over  $\mathbb{R}$  such that  $b_{kl} \ge 0$  for  $k \ne l$  and  $\sum_{l=1}^{n} b_{kl} = 0$ for k = 1, 2, ..., m is called an *intensity matrix*. An intensity matrix C is called an *extreme intensity matrix* if C has only one nonzero off-diagonal element which is equal to 1. An extreme intensity matrix  $C = ||c_{kl}||$  is denoted by  $E_{pq}$   $(p \ne q)$  if  $c_{pp} = -1$  and  $c_{pq} = 1$ .

It is easy to see that the set of all non-singular  $n \times n$  stochastic matrices forms a subsemigroup of  $GL(n, \mathbb{R})$ .

**Lemma 2.1.** Let  $S_n$  be the semigroup of all real  $n \times n$  non-singular matrices with non-negative entries. Then  $\mathscr{D}(S_n)$  coincides with the set of all real  $n \times n$  matrices which are non-negative off the diagonal.

Proof. Let  $A = ||a_{ij}|| \in \mathscr{D}(S_n)$ . Then  $A = (\frac{\mathrm{d}X(t)}{\mathrm{d}t})|_{t=0}$  with  $X(t) \in S_n$  for each t and X(0) = I. Since  $X(t) \in S_n$ ,  $x_{ij}(t) \ge 0$  for  $i, j = 1, 2, \ldots n$ . From X(0) = I,  $x_{ij}(0) = 0$  for  $i \ne j$ . Thus  $a_{ij} = (\frac{\mathrm{d}x_{ij}(t)}{\mathrm{d}t})|_{t=0} \ge 0$  for  $i \ne j$ .

Conversely let  $E_{ij}(i \neq j)$  be an extreme intensity matrix as denoted in the above definition. Since  $E_{ij}^2 = -E_{ij}$ ,  $\exp(tE_{ij}) = I + tE_{ij} - \frac{t^2}{2!}E_{ij} + \frac{t^3}{3!}E_{ij} + \ldots = I + (1 - e^{-t})E_{ij}$ , and hence  $\exp(tE_{ij}) \in S_n$  for  $t \ge 0$ . Since  $E_{ij} = \frac{d}{dt}(\exp(tE_{ij}))|_{t=0}$ ,

 $E_{ij} \in \mathscr{D}(S_n)$ . Let  $E_k$  be the matrix whose elements are 0 except that the k-th diagonal element is equal to 1. Since  $E_k^2 = E_k$ ,  $\exp(tE_k) = I + tE_k + \frac{t^2}{2!}E_k + \frac{t^3}{3!}E_k + \ldots = I + (e^t - 1)E_k$ , and hence  $\exp(tE_k) \in S_n$  for  $t \ge 0$ . Thus  $E_k \in \mathscr{D}(S_n)$ . Similarly we may show  $-E_k \in \mathscr{D}(S_n)$ . Since  $\mathscr{D}(S_n)$  forms a convex cone in the matrix space  $gl(n, \mathbb{R})$ ,  $\sum_{1 \le i \ne j \le n} \alpha_{ij}E_{ij} + \sum_{k=1}^n \beta_k E_k - \sum_{k=1}^n \gamma_k E_k \in \mathscr{D}(S_n)$  for all  $\alpha_{ij}$ ,  $\beta_k, \gamma_k \ge 0$ . Thus every real  $n \times n$  matrix which is non-negative off the diagonal is contained in  $\mathscr{D}(S_n)$ .

**Lemma 2.2.** Let  $T_n$  be the semigroup of all real non-singular  $n \times n$  matrices with each row sum equal to 1. Then

$$\mathscr{D}(T_n) = \bigg\{ \|c_{ij}\| \in gl(n, \mathbb{R}) \colon \sum_{j=1}^n c_{ij} = 0 \text{ for } i = 1, 2, \dots, n \bigg\}.$$

Proof. Let  $\Omega = \|\omega_{ij}\| \in \mathscr{D}(T_n)$ . Then there exists  $U(t) \in T_n$  such that  $\Omega = \left(\frac{dU(t)}{dt}\right)|_{t=0}, \sum_{j=1}^n u_{ij}(t) = 1$  for i = 1, 2, ..., n, and U(0) = I. Hence

$$\sum_{j=1}^{n} \omega_{ij} = \sum_{j=1}^{n} \frac{\mathrm{d}}{\mathrm{d}t} (u_{ij}(t))|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t} \left( \sum_{j=1}^{n} u_{ij}(t) \right) \Big|_{t=0}$$
$$= \frac{\mathrm{d}}{\mathrm{d}t} (1) \Big|_{t=0} = 0 \quad \text{for } i = 1, 2, \dots, n.$$

Conversely suppose that  $C = ||c_{ij}||$  with  $\sum_{j=1}^{n} c_{ij} = 0$  for i = 1, 2, ..., n. Let

$$W = \bigg\{ \|b_{ij}\| \in gl(n, \mathbb{R}) \colon \sum_{j=1}^{n} b_{ij} = 0 \text{ for } i = 1, 2, \dots, n \bigg\}.$$

Then W is a cone in  $gl(n, \mathbb{R})$  and  $C \in W$ . Also

$$C = \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{tC} \Big|_{t=0} = \lim_{t \to 0^+} \frac{\mathrm{e}^{tC} - I}{t}.$$

Since  $C \in W$  and W is a cone,  $\exp(tC) \in I + tW = I + W$  for  $t \ge 0$ . Since  $\exp(tC)$  is non-singular,  $\exp(tC) \in \operatorname{GL}(n, \mathbb{R}) \cap (I + W) \subset T_n$ . Thus  $C \in \mathscr{D}(T_n)$ .

**Lemma 2.3.** Let  $S_n$  be the semigroup of all  $n \times n$  non-singular stochastic matrices. Then  $\Omega = ||\omega_{ij}||$  is an element of  $\mathscr{D}(S_n)$  iff  $\Omega$  is an  $n \times n$  intensity matrix.

Proof. It is clear that if  $S_n$  and  $T_n$  are subsemigroups of  $GL(n, \mathbb{R})$ , then  $\mathscr{D}(S_n \cap T_n) = \mathscr{D}(S_n) \cap \mathscr{D}(T_n)$ . Thus the lemma is proved from Lemma 2.1 and Lemma 2.2.

**Theorem 2.4.** Let  $S_n$  be the semigroup of all  $n \times n$  non-singular upper (or lower) triangular stochastic matrices. Then A is an element of  $\mathscr{D}(S_n)$  iff A is an  $n \times n$  upper (or lower) triangular intensity matrix.

Proof. It is obvious that if  $T_n$  is the semigroup of all real  $n \times n$  non-singular upper (or lower) triangular matrices, A is an element of  $\mathscr{D}(T_n)$  iff A is a real  $n \times n$  upper (or lower) triangular matrix. Hence the theorem is proved from Lemma 2.3.

#### 3. Infinitesimally generated triangular stochastic matrices

**Lemma 3.1.** Let A be an  $n \times n$  non-singular upper triangular stochastic matrix of the following form:

	(1)	0		0	0	0		0 \	
A =	0	1		0	0	0		0	
	1	÷	·.	÷	÷	÷	÷	:	
	0	0		1	0	0		0	
		Δ		Ω	a	0 1		a	•
	0	0		0	$u_{pp}$	app+1	• • •	$a_{pn}$	
	0	0	· · · · · · ·	0	$0^{a_{pp}}$	$\frac{\alpha_{pp+1}}{1}$		$\begin{bmatrix} a_{pn} \\ 0 \end{bmatrix}$	
	0	0 :	••••	0 :	$egin{array}{c} u_{pp} \ 0 \ dots \end{array}$	$egin{array}{c} \vdots \\ 0 \\ a_{pp+1} \\ 1 \\ \vdots \end{array}$	···· ···	$\begin{bmatrix} a_{pn} \\ 0 \\ \vdots \end{bmatrix}$	

Then A can be represented as  $A = \exp(t_{pp+1}E_{pp+1})\exp(t_{pp+2}E_{pp+2})\dots\exp(t_{pn}E_{pn})$ , where  $E_{ij}$  is an extreme intensity matrix as denoted in the definition of Section 2.

Proof. Since A is stochastic,  $a_{pp} + a_{pp+1} + \ldots + a_{pn} = 1$ . Since A is upper triangular and non-singular, determinant of  $A = a_{pp} > 0$ . Let

$$x_{p+i} = \frac{a_{pp} + a_{pp+i+1} + \ldots + a_{pn}}{a_{pp} + a_{pp+i} + \ldots + a_{pn}} \text{ for } i = 1, 2, \dots, n.$$

Then  $0 < x_{p+i} \leq 1$  for i = 1, 2, ..., n since  $a_{pp} > 0$ . For  $i = 1, x_{p+1} = a_{pp} + a_{pp+2} + ... + a_{pn}$ . Thus  $a_{pp+1} = 1 - x_{p+1}$ . Now,

$$x_{p+2} = \frac{a_{pp} + a_{pp+3} + \ldots + a_{pn}}{a_{pp} + a_{pp+2} + \ldots + a_{pn}} = \frac{a_{pp} + a_{pp+3} + \ldots + a_{pn}}{x_{p+1}}$$

Hence  $a_{pp+2} = x_{p+1} - x_{p+1}x_{p+2} = x_{p+1}(1 - x_{p+2})$ . Inductively,

$$x_{p+1}x_{p+2}\dots x_{p+k-1} = a_{pp} + a_{pp+k} + \dots + a_{pn}$$

252

for  $k = 2, \ldots, n - p$  and

$$x_{p+1}x_{p+2}\dots x_{p+k-1}x_{p+k} = a_{pp} + a_{pp+k+1} + \dots + a_{pn}$$

Therefore

$$a_{pp+k} = x_{p+1} \dots x_{p+k-1} (1 - x_{p+k})$$
 for  $k = 2, \dots, n-p$ .

We have

$$1 = a_{pp} + a_{pp+1} + a_{pp+2} + \ldots + a_{pn}$$
  
=  $a_{pp} + (1 - x_{p+1}) + x_{p+1}(1 - x_{p+2}) + \ldots + x_{p+1} \ldots x_{n-1}(1 - x_n)$   
=  $a_{pp} + 1 - x_{p+1} \ldots x_n$ .

Hence  $a_{pp} = x_{p+1}x_{p+2}...x_n$ . Let  $A_{x_{p+j}}$  (j = 1, 2, ..., n-p) be an  $n \times n$  upper triangular stochastic matrix of the following form:

$$A_{x_{p+j}} = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \dots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots & \vdots & \ddots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots & 1 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots & \vdots & \ddots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & \dots & 1 \end{pmatrix},$$

where  $x_{p+j}$  is in the *p*th low and *p*th column and  $1 - x_{p+j}$  is in the *p*th low and p + jth column. Then  $A = A_{x_{p+1}}A_{x_{p+2}} \dots A_{x_n}$ . Since  $0 < x_{p+j} \leq 1$ ,  $A_{x_{p+j}} = \exp(t_{pp+j}E_{pp+j})$  for some  $t_{pp+j} \geq 0$ . Thus  $A = \exp(t_{pp+1}E_{pp+1})\exp(t_{pp+2}E_{pp+2}) \dots \exp(t_{pn}E_{pn})$ .

**Lemma 3.2.** If U is an  $n \times n$  non-singular upper triangular stochastic matrix, then it can be represented as  $U = C_{n-1}C_{n-2}\ldots C_1$ , where  $C_p = \exp(t_{pp+1}E_{pp+1})\ldots$  $\exp(t_{pn}E_{pn})$  for  $p = 1, 2, \ldots, n-1$  and  $t_{ij} \ge 0$ .

Analogously, if L is an  $n \times n$  non-singular lower triangular stochastic matrix, then it can be represented as  $L = H_2H_3...H_n$ , where  $H_p = \exp(s_{p1}E_{p1})\exp(s_{p2}E_{p2})...$  $\exp(s_{pp-1}E_{pp-1})$  for p = 2,...,n and  $s_{ij} \ge 0$ . Proof. Let  $U_1, \ldots, U_n$  be the rows of U such that  $U = (U_1, \ldots, U_n)^t$  and  $I_j$  be the *j*th row of  $n \times n$  identity matrix. Then  $U = C_{n-1}C_{n-2}\ldots C_1$ , where  $C_p$  is an  $n \times n$  matrix such that  $C_p = (I_1, I_2, \ldots, I_{p-1}, U_p, I_{p+1}, \ldots, I_n)^t$  for  $p = 1, 2, \ldots, n-1$ . According to the Lemma 3.1,  $C_p = \exp(t_{pp+1}E_{pp+1})\ldots\exp(t_{pn}E_{pn})$ .

The proof for the lower triangular case is similar to that for the upper triangular case.  $\hfill \square$ 

**Theorem 3.3.** Each element in the semigroup  $S_n$  of all  $n \times n$  non-singular upper (or lower) triangular stochastic matrices is generated from the infinitesimal elements of  $S_n$ , which form a cone consisting of all  $n \times n$  upper (or lower) triangular intensity matrices.

Proof. Immediate from Theorem 2.4 and Lemma 3.2.

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