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# Total positivity and the embedding problem for Markov chains

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*Abstract*

We prove that the class of transition matrices for the finite state time-inhomogeneous birth and death processes coincides with the class of non-singular totally positive stochastic matrices. Thus we obtain a complete solution to the embedding problem for this class of Markov chains.

## 1. *Introduction*

A non-singular stochastic matrix $P$ will be called embeddable if there exists a two-parameter family of stochastic matrices

$$\{P(s,t)\ 0 \leqslant s \leqslant t < +\infty\}$$

satisfying
$$P(s,t) = P(s,u)\,P(u,t) \quad (0 \leqslant s \leqslant u \leqslant t), \tag{1}$$

$$\lim_{t \downarrow s} P(s,t) = \lim_{s \uparrow t} P(s,t) = I \tag{2}$$

and such that
$$P(0,1) = P. \tag{3}$$

The problem of characterizing the embeddable stochastic matrices has proven to be quite difficult at the level of generality of (3). The most extensive and useful characterizations to date have been by Johansen(2), (3) and Kingman(7). For our purposes we will require a reformulation of the embedding problem as a control problem for differential equations – discussed in detail in Johansen(2), (3). The essential point is that a non-singular stochastic matrix $P$ is embeddable if and only if there is a two-parameter family of absolutely continuous matrix functions $\{P(s,t),\ 0 \leqslant s \leqslant t < +\infty\}$ satisfying (2),

$$\frac{\partial}{\partial t} P(s,t) = P(s,t)\,Q(t) \quad (t \notin N), \tag{4}$$

$$\frac{\partial}{\partial s} P(s,t) = -Q(s)\,P(s,t) \quad (s \notin N), \tag{5}$$

where $N$ is a null set, and such that $P(0,1) = P$. For each $t \geqslant 0$,

$$Q(t) \in \mathbf{Q}_0 = \left\{Q: q_{ii} \leqslant 0, q_{ij} \geqslant 0, i \neq j, \sum_{j=1}^{n} q_{ij} = 0\right\},$$

the class of intensity matrices. Thus $P$ can be embedded if it can be reached via (4) and (5) using a bounded measurable controller $Q(.) \in \mathbf{Q}_0$.

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In this paper we restrict attention to the finite state birth and death processes; that is, the continuous-time Markov chains whose transition probabilities are governed by (4) and (5) with $Q(t) \in \mathbf{Q}_1 = \mathbf{Q}_0 \cap \{Q: q_{ij} = 0 \text{ if } |i-j| > 1\}$ – the class of Jacobi intensity matrices. For the time-homogeneous birth and death processes – i.e. $Q(t) \equiv$ constant $= Q^{\cdot} \in \mathbf{Q}_1$ – Karlin and McGregor (6) proved that the transition matrices

$$P(s,t) = P(t-s) = e^{(t-s)Q^{\cdot}} \quad (0 \leqslant s \leqslant t < +\infty) \tag{6}$$

are totally positive. Recall that a matrix $A = \|a_{ij}\|$ is called *totally positive* – hereafter abbreviated $TP$ – if for any $i_1 < \ldots < i_k$ and $j_1 < \ldots < j_k$

$$\det \begin{vmatrix} a_{i_1,j_1} \ldots a_{i_1,j_k} \\ \vdots \qquad\quad \vdots \\ a_{i_k,j_1} \ldots a_{i_k,j_k} \end{vmatrix} \geqslant 0 \quad (k = 1, 2, \ldots, n). \tag{7}$$

Although (7) is a necessary condition for embeddability in the time-homogeneous birth and death processes, it is easy to verify that the inclusions

$$\begin{aligned} &P_0 = \{\text{time-homogeneous birth and death transition matrices}\}, \\ \subset\ &P_1 = \{\text{time-homogeneous embeddable } TP \text{ matrices}\}, \\ \subset\ &TP \text{ nonsingular stochastic matrices} \end{aligned}$$

are proper. Now let

$P_2 = \{\text{time-inhomogeneous birth and death transition matrices}\} = \{P: P \text{ can be reached from the identity using a bounded measurable controller } Q(.) \in \mathbf{Q}_1\}$.

The purpose of this paper is to prove

THEOREM 1. *$P_2 = TP$ non-singular stochastic matrices.*

An interesting feature of our results for birth and death processes in comparison with the general embedding problem is that the set of *all* non-singular $TP$ stochastic matrices admit a representation as a *finite* product of exponentials of extreme *Jacobi* intensity matrices. Johansen (3) proves that any matrix in the *interior* of the set of embeddable matrices – i.e. those satisfying (3) – admits a representation as a finite product of extreme intensity matrices. A satisfactory characterization of the boundary of the general embeddable matrices remains to be carried out.

To fix our terminology, let $Q_{ij}$ $(i \neq j)$ denote the extreme intensity matrix with elements

$$[Q_{ij}]_{mk} = \begin{cases} -1 & \text{if } i = m = k \\ 1 & \text{if } m = i, j = k. \\ 0 & \text{otherwise} \end{cases}$$

$Q_{ij}$ $(i \neq j)$ is called an extreme *Jacobi* intensity matrix if $|j-i| = 1$. Let

$$[E_{ij}]_{mk} = \begin{cases} 1 & \text{if } m = i,\ k = j \\ 0 & \text{otherwise.} \end{cases}$$

A Poisson matrix $e^{\lambda Q_{ij}} = I - (1-e^{-\lambda}) E_{ii} + (1-e^{-\lambda}) E_{ij}$, $\lambda > 0$, is called a Jacobi Poisson matrix if $|i-j| = 1$. Finally, let

$$a_{ij} = 1 - e^{-\lambda}$$

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and $$A(a_{ij}) = I - a_{ij}E_{ii} + a_{ij}E_{ij}.$$

In terms of these ingredients we prove,

THEOREM 1'. *If $P$ is an $n \times n$ non-singular, stochastic $TP$ matrix, then it can be represented as*

$$P = B_1 B_2 \dots B_{n-1} C_1 C_2 \dots C_{n-1}, \tag{8}$$

where $B_i$ and $C_i$ are of the form

$$B_i = A_{n,n-1}(a^i_{n,n-1})\, A_{n-1,n-2}(a^i_{n-1,n-2}) \dots A_{i+1,i}(a^i_{i+1,i}), \tag{9}$$

$$C_i = A_{n-i,n-i+1}(a^{n-i}_{n-i,n-i+1})\, A_{n-i+1,n-i+2}(a^{n-i}_{n-i+1,n-i+2}) \dots A_{n-1,n}(a^{n-i}_{n-1,n}), \tag{10}$$

$$0 \leqslant a^i_{kl} < 1 \quad (1 \leqslant i < n).$$

The specification of $a^i_{kl}$ will become evident from the proof.

2. *Proof of Theorem* 1

(A) *Necessity.* If $P$ is embeddable it can be represented as a product integral

$$P = \prod_0^1 [I + Q(t)\,dt], \tag{11}$$

where $Q(.)$ is a bounded measurable Jacobi-matrix-valued function. (See, for example, Johansen(2), pp. 186–189; Gantmacher(1), pp. 131–135, and Schlesinger(8) for details on product integrals.) Introduce the matrix norm, $\|A\| = \sup_i \sum_j |a_{ij}|$, and recall that $\forall$ Jacobi intensity matrix $Q$, $I + \epsilon Q \in TP$ for $\epsilon$ sufficiently small (see, for example, Karlin(5), p. 115). Since $Q(.)$ is bounded, $\exists\ \epsilon^*$ such that for $\epsilon < \epsilon^*$

$$I + \epsilon Q(t) \in TP \quad \forall\, t \geqslant 0.$$

Consider the partitions

$$\Pi^* = (\{t_i\}_{i=0}^n : 0 = t_0 < t_1 \dots < t_n = 1 \text{ such that } \max_{0 \leqslant i \leqslant n} (t_{i+1} - t_i) < \epsilon^*).$$

By the definition of product integral, $\forall \epsilon_1 > 0$, $\exists N(\epsilon_1)$ such that if $n \geqslant N(\epsilon_1)$,

$$\Big\| \prod_0^1 [I + Q(t)\,dt] - \prod_0^{n-1} [I + (t_{i+1} - t_i)\, Q(t_i)] \Big\| < \epsilon_1,$$

where $\{t_i\}_{i=0}^n \in \Pi^*$. Since the class of $TP$ matrices is closed under matrix multiplication,

$$\prod_0^{n-1} [I + (t_{i+1} - t_i)\, Q(t_i)] \in TP.$$

Since $\epsilon_1$ is arbitrary $P = \prod_0^1 (I + Q(t)\,dt) \in TP$, as claimed.

(B) *Sufficiency* (Proof of Theorem 1'). Let

$$a^1_{k,k-1} = \begin{cases} \dfrac{p_{k,1}}{p_{k-1,1}} & \text{for} \quad k = 2, \dots, l = \max\,(k : p_{k,1} > 0) \\ 0 & \text{for } k = l+1, \dots, n. \end{cases}$$

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We require the following lemma.

LEMMA 1. *If $P \in TP$ is non-singular and stochastic then*

$$a^1_{k,k-1} < 1 \quad (k = 2, \ldots, n).$$

*Proof.* Assume that $a^1_{m,m-1} \geqslant 1$ for some $m$, where $2 \leqslant m \leqslant n$. Then $P \in TP$ implies

$$0 \leqslant \begin{vmatrix} p_{m-1,1} & p_{m-1,j} \\ p_{m,1} & p_{m,j} \end{vmatrix} = p_{m-1,1}(p_{m,j} - p_{m-1,j} a^1_{m,m-1}). \tag{12}$$

Combining (12) with the inequality $a^1_{m,m-1} \geqslant 1$ yields

$$p_{m,j} \geqslant p_{m-1,j} \quad \text{for} \quad j = 1, \ldots, n.$$

But this is impossible since $P$ is both stochastic and non-singular.

We establish the representation (8) by an elimination argument. For elements below the diagonal we begin with the $(n, 1)$ entry in $P$ and work upwards to the $(2, 1)$ entry through the sequence of factorizations

$$P = U_{k+1,1} V_{k,1} \quad \text{for} \quad k = n-1, n-2, \ldots, 1$$

where $U_{k+1,1}$ is the product of Jacobi–Poisson matrices,

$$U_{k+1,1} = A_{n,n-1}(a^1_{n,n-1}) \ldots A_{k+1,k}(a^1_{k+1,k})$$

and where $V_{n,1} \equiv P$. As verified below, $V_{k,1}$ is a $TP$ stochastic matrix with $v_{n,1} = \ldots = v_{k+1,1} = 0$.

Setting $V_{n,2} \equiv V_{1,1}$, we continue the elimination with the $(n, 2)$ entry in $V_{n,2}$ working upward through columns 2, 3, ..., $n-1$, respectively, via the factorizations

$$P = U_{k+1,j} V_{k,j} \quad (n-1 \geqslant k \geqslant j).$$

At each change of column we set $V_{n,j+1} \equiv V_{j,j}$. Here,

$$U_{k+1,j} = B_1 \ldots B_{j-1} A_{n,n-1}(a^j_{n,n-1}) \ldots A_{k+1,k}(a^j_{k+1,k}),$$

where $B_i$, given by (9), results from eliminations in column $i$; and $V_{k,j}$ is a $TP$ stochastic matrix with $v_{m,i} = 0$ for $n \geqslant m > i = 1, 2, \ldots, j-1$ and $(m, i) = (n, j), \ldots, (k+1, j)$. The entries in the Jacobi Poisson matrices are defined by

$$a^j_{k+1,k} = \begin{cases} \dfrac{v_{k+1,j}}{v_{k,j}} & \text{from the matrix } V_{k+1,j} \text{ provided } v_{k+1,j} > 0 \\ 0 & \text{if the } (k+1, j) \text{ entry in } V_{k+1,j} \text{ is zero.} \end{cases}$$

That $a^j_{k+1,k} < 1$ follows from the same argument used in the proof of Lemma 1.

The above elimination of elements under the diagonal finally yields the representation

$$P = B_1 B_2 \ldots B_{n-1} T,$$

where $T$ is upper triangular, stochastic, and $TP$. To complete the construction of (8), we begin with the $(1, n)$ entry in $T \equiv T_{1,n}$ and work across the first row to the (1, 2) entry via the factorizations

$$T = T_{1,n-k} A_{n-k,n-k+1}(a^{n-1}_{n-k,n-k+1}) \ldots A_{n-1,n}(a^{n-1}_{n-1,n}),$$

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where $T_{1,n-k}, k = 1, 2, \ldots, n-1$ are $TP$ stochastic with $t_{1,n-j+1} = 0$ for $j = 1, 2, \ldots, k$; and

$$a^{n-1}_{n-k,n-k+1} = \left\{ \begin{array}{ll} \dfrac{t_{1,n-k+1} + \ldots + t_{1,n}}{t_{1,n-k} + \ldots + t_{1,n}} & \text{from the matrix } T_{1,n-k+1} \text{ provided } t_{1,n-k+1} > 0 \\ 0 & \text{otherwise.} \end{array} \right\} \tag{13}$$

We continue the elimination with the $(2, n)$ entry in $T_{1,1} \equiv T_{2,n}$ and work through rows 2, 3, ..., $n-1$ via the factorizations

$$T = T_{j,n-k} A_{n-k,n-k+1}(a^{n-j}_{n-k,n-k+1}) \ldots A_{n-1,n}(a^{n-j}_{n-k,n}) C_{n-j+1} \ldots C_{n-1}$$

where $\{C_i\}_{i=1,\ldots,n-1}$ are given by (10). The entries $a^{n-j}_{n-k,n-k+1}$ are defined analogous to (13) from the $TP$ stochastic matrix $T_{j,n-k+1}$. These above-diagonal eliminations finally yield $T = C_1 C_2 \ldots C_{n-1}$, thereby establishing (8).

We verify that $\{V_{k,j}\}_{k \geqslant j}$ and $\{T_{j,n-k}\}_{n-k \geqslant j}$ are $TP$ stochastic by an induction argument on the order of sub-determinants within each matrix, as well as by induction on the elimination step. To this end, let $r_1, \ldots, r_n$ be the rows of $P = (r_1, \ldots, r_n)$ and define a positive row operation to be any combination of

(i) $(r_1, \ldots, r_n) \to (r_1, \ldots \lambda r_i, r_{i+1} \ldots, r_n) \quad (\lambda > 0)$,

(ii) $(r_1, \ldots, r_n) \to (r_1, \ldots, r_{i-1}, r_i \pm r_{i-1}, r_{i+1}, \ldots, r_n)$.

Clearly (i) preserves $TP$ while (ii) preserves the sign of all sub-determinants of order 2 or more based on consecutive rows and arbitrary ordered columns. Now set

$$l = \max (k : p_{k\,1} > 0)$$

and observe that $V_{l-1,1}$ is derived from $P$ by positive row operations which also preserve non-negativity of the entries. In particular

$$V_{l-1,1} = (r_1, \ldots, r_{l-1}, \lambda_2 r_l - \lambda_1 r_{l-1}, r_{l+1}, \ldots, r_n),$$

where $$\lambda_1 = \frac{p_{l,1}}{p_{l-1,1} - p_{l,1}} \quad \text{and} \quad \lambda_2 = \frac{p_{l-1,1}}{p_{l-1,1} - p_{l,1}}.$$

We call an $n \times n$ matrix $TP_m$ if its entries and all minors of order $j \leqslant m$ are non-negative; it is called $TP$ if it is $TP_m$ for $m = 1, 2, \ldots, n$. Since $V_{l-1,1} \in TP_1$, we assume, for the induction step, that it is also in $TP_{m-1}$. Then we require

LEMMA 2 (Fekete, see, for example, (5), p. 59). *If an $n \times n$ matrix $(n \geqslant m)$ has all its minors of order $m-1$ which come from the last $m-1$ columns and all $m$th order minors which come from consecutive rows positive, then all $m$th order minors are positive.*

Since any $TP_{m-1}$ matrix may be approximated arbitrarily closely elementwise by a strictly $TP_{m-1}$ matrix (see, for example, (9), p. 88) we apply Lemma 2 to $V^{(\epsilon)}$, which approximates $V_{l-1,1}$ thereby establishing that $V^{(\epsilon)}$ is strictly $TP_m$. Letting $\epsilon \to 0$, $V^{(\epsilon)} \to V_{l-1,1}$ and we have that $V_{l-1,1} \in TP_m$. Since $m$ may be any integer $\leqslant n$, $V_{l-1,1} \in TP$. The identical argument verifies that $V_{k,j} \in TP$ for $k \geqslant j$.

Finally, since $T_{j,n-k}$ is derived from $T_{j,n-k+1}$ by positive column operations – analogous to the row operations (i) and (ii) – the above perturbation argument and Fekete's lemma with the role of rows and columns interchanged can be applied to verify that $\{T_{j,n-k}\}_{n-k \geqslant j}$ are $TP$.

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*Note added in proof:* The implication that (1) and (2) imply (4) and (5) is originally due to GOODMAN, G. S. *Z. Wahr.* **16**, (1970), 165–180.

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