Z. Wahrscheinlichkeitstheorie verw. Gebiete
53, 305–316 (1980)

Zeitschrift für
Wahrscheinlichkeitstheorie
und verwandte Gebiete

A Structure of the Bang-Bang Representation for 3×3 Embeddable Matrices

Halina Frydman*

524 Tish Hall, New York University, Washington Square, New York, N.Y. 10003, USA

Summary. Necessary and sufficient conditions are given for a 3×3 stochastic matrix to be embeddable by 6 elementary stochastic matrices (Poisson matrices). For a 3×3 embeddable matrix, a structure of the minimal Bang-Bang representation, i.e. the one that contains the smallest number of elementary matrices, is obtained. Based on the minimal Bang-Bang representation an algorithm for determining the embeddability of a 3×3 stochastic matrix is given.

1. Introduction, Survey of Results, and Summary

We consider the embedding problem for Markov chains with three states. A nonsingular stochastic matrix P is called embeddable if there exists a two-parameter family of stochastic matrices

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

satisfying $P(s,t)=P(s,u)P(u,t) \qquad (0\leqq s\leqq u\leqq t)$,

$$\lim_{t\downarrow s} P(s,t)=\lim_{s\uparrow t} P(s,t)=I \tag{1.1}$$

and such that $P(0,1)=P$.

The embedding problem was reformulated by Goodman [3] as a control problem for differential equations. Goodman showed that a nonsingular stochastic matrix P is embeddable if and only if there is a two-parameter family of absolutely continuous matrix functions $\{P(s,t),\ 0\leqq s\leqq t<+\infty\}$ *satisfying* (1.1).

$$\frac{\partial}{\partial t} P(s,t)=P(s,t)\,Q(t) \qquad (t\notin N), \tag{1.2}$$

* I would like to thank Søren Johansen for helpful comments and stimulating discussions on the subject of this paper

0044-3719/80/0053/0305/$02.40

$$\frac{\partial}{\partial s} P(s,t) = -Q(s)P(s,t) \qquad (s \notin N) \tag{1.3}$$

where N is a null set, and such that $P(0,1)=P$.

For each $t \geqq 0$

$$Q(t) \in Q_0 = \left\{ Q\colon q_{ii} \leqq 0,\ q_{ij} \geqq 0,\ i \neq j,\ \sum_{j=1}^{n} q_{ij} = 0 \right\}$$

the class of intensity matrices.

The embeddable matrices are thus the matrices that can be reached from the identity I via (1.2) and (1.3) using a suitable controller $Q(\cdot) \in Q_0$. The intensity matrices form a convex cone and the extremal elements have at most one positive off-diagonal element. A stochastic matrix which can be reached via (1.2) or (1.3) using an extremal intensity matrix Q as a controller is called a Poisson matrix and is of the form $e^{\lambda Q}$, $\lambda > 0$.

Applying the chattering principle from control theory, see [8], to the control system specified by (1.1), (1.2) and (1.3), Johansen [4] formulated the following characterization of embeddable matrices: any embeddable matrix can be approximated by a finite product of Poisson matrices. Johansen [5] further proved that any matrix in the interior of the set of embeddable matrices has a representation as a finite product of Poisson matrices, i.e., it has a Bang-Bang representation.

Frydman and Singer [2] obtained the complete solution to the embedding problem for the birth and death processes. They showed that the class of transition matrices for birth and death processes coincides with the class of non-singular totally positive stochastic matrices and that *all* transition matrices of birth and death processes admit a Bang-Bang representation.

For 3×3 stochastic matrices Johansen [5] proved, using geometric methods, that matrices on the boundary of the set of embeddable matrices admit a Bang-Bang representation, see also Frydman [1] for an algebraic proof. Characterization of the boundary of the general embeddable matrices is an open problem.

This paper relies heavily on methods and results in [1]. We will briefly summarize results in [1] needed here after we introduce the necessary notation.

Notation. Throughout this paper we will refer to a 3×3 stochastic matrix P as "a matrix P." We will denote by $P > 0$ a matrix with all elements positive, and by $P \geqq 0$ a matrix with at least one off-diagonal element equal to zero.

Let $S = \{(i,j,k) | (i,j,k)$ is a permutation of $(1,2,3)\}$ and let

$$\begin{aligned} T_{ij} &= p_{ji} p_{kk} - p_{jk} p_{ki} \\ T_{ii} &= p_{jj} p_{kk} - p_{jk} p_{kj} \end{aligned} \qquad (i,j,k) \in S.$$

Note that

$$\begin{aligned} T_{ij} &= (-1)^{i+j-1} M_{ij} \\ T_{ii} &= M_{ii} \end{aligned}$$

where M_{ij}, M_{ii} are second order minors of P. Observe that for every $(i,j,k) \in S$

$$\det P = p_{kk} T_{kk} - p_{jk} T_{jk} - p_{ik} T_{ik} = p_{jj} T_{jj} - p_{jk} T_{jk} - p_{ji} T_{ji}.$$

Let E_{ij} be a matrix with elements

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

and $A_{ij}(u)$ denote the following Poisson matrix

$$A_{ij}(u)=I-uE_{ii}+uE_{ij}, \qquad 0\leqq u<1.$$

Let $c=\frac{u}{1-u}$. We denote by $Z_{ij}(c)$ the inverse of $A_{ij}(u)$, i.e.,

$$Z_{ij}(c)=I+cE_{ii}-cE_{ij}, \qquad c=\frac{u}{1-u}\geqq 0.$$

Let the stochastic matrix P have columns (p_1, p_2, p_3) and let $P_1=PZ_{ij}(c)$. Then a simple calculation gives

$$p_k^{(1)}=\begin{cases}p_k & \text{if } k\neq i,j\\ p_j-cp_i & \text{if } k=j\\ p_i(1+c) & \text{if } k=i\end{cases} \tag{1.4}$$

$$\det P_1=(1+c)\det P.$$

Note that $P_1=\|p_{ij}^{(1)}\|$ satisfies $\sum_{j=1}^{3} p_{ij}^{(1)}=1;\ 1\leqq i\leqq 3$ but may not be stochastic.

It was shown by Goodman [3] that $\prod_{i=1}^{n} p_{ii}\geqq\det P>0$ is a necessary condition for embeddability of an $n\times n$ stochastic matrix P. For $n=3$ we proved in [1].

Theorem 1.1. *$\prod_{i=1}^{3} p_{ii}\geqq\det P>0$ is a sufficient and necessary condition for embeddability of a matrix $P\geqq 0$ and in this case $P=\prod_{m=1}^{5} A_m$ where $(A_m,\ 1\leqq m\leqq 5)$ are Poisson matrices.*

A similar result does not hold for $n>3$, see Kingman and Williams [7].

For $P>0$ let

$$B(n,m)=p_{nn}p_{mm}\frac{T_{nm}}{p_{mn}}, \qquad n,m=1,2,3,$$

$$B(P)=\max_{(n,m)} B(n,m)$$

and

$$\bar{c}_{ij}=\min\left(\frac{p_{ij}}{p_{ii}}, \frac{p_{kj}}{p_{ki}}, \frac{p_{jj}}{p_{ji}}\right), \qquad (i,j,k)\in S.$$

The following two lemmas show the significance of the function $B(P)$ for the embedding problem.

Lemma 1.1. *Let $P=\prod_{m=1}^{l} A_m>0$ and assume that $B(P)<\det P$. Then also $PA_l^{-1}>0$.*

In what follows $p_{ij}^{(m)}$ denotes the (i,j)'th element of a matrix P_m;

$$T_{ij}^{(m)} = p_{ji}^{(m)} p_{kk}^{(m)} - p_{jk}^{(m)} p_{ki}^{(m)} \quad \textit{and} \quad B_m(i,j) = p_{ii}^{(m)} p_{jj}^{(m)} \frac{T_{ij}^{(m)}}{p_{ji}^{(m)}}.$$

We call a matrix P *regular* if all its principal minors are positive, i.e., if $T_{ii} > 0$ for all $1 \leqq i \leqq 3$.

Lemma 1.2. *Suppose* $P > 0$, $\det P > 0$, *and* $B(P) < \det P$. *Let* $P_1 = PZ_{ij}(c)$ *where* $(i,j,k) \in S$ *and* $0 < c < \bar{c}_{ij}$ *so that* $P_1 > 0$. *Then*

a) $B_1(n,m) < \det P_1$ *for all* $(n,m) \neq (j,i)$;

b) *If* P *is regular*, $B(P_1) < \det P_1$.

These lemmas and Theorem 1.1 were used to prove

Theorem 1.2. *For a positive matrix* P

a) $B(P) \geqq \det P > 0$ *is a sufficient condition for embeddability of* P *by at most* 6 *Poisson matrices and the structure of the embedding product is one of the following:*

$$P = A_{ki} A_{jk} A_{kj} A_{ik} A_{ji} A_{ij}, \qquad P = A_{ji} A_{jk} A_{kj} A_{ik} A_{ji} A_{kj}, \qquad \textit{or}$$
$$P = A_{ki} A_{jk} A_{kj} A_{ik} A_{ji} A_{kj} \qquad \textit{for some } (i,j,k) \in S.$$

b) *If* P *is regular and* $P = \prod_{m=1}^{6} A_m$ *then* $B(P) \geqq \det P > 0$.

With this background we can summarize the main results of this paper. The main result of section 2 is the characterization of 3×3 stochastic matrices embeddable by at most 6 Poisson matrices. For a positive 3×3 stochastic matrix P a necessary and sufficient condition to be embeddable by at most 6 Poisson matrices is

$$B(i,j) \equiv p_{ii} p_{jj} \frac{T_{ij}}{p_{ji}} \geqq \det P > 0 \qquad \text{for some } i,j = 1,2,3$$

or that $\exists (i,j,k) \in S$ and $0 < c < \bar{c}_{ij}$ such that

$$B_1(j,i) = \det P_1 \qquad \text{where } P_1 = PZ_{ij}(c). \tag{1.5}$$

Equation (1.5) is equivalent to the following quadratic equation in c:

$$p_{ji} p_{ii} T_{jj} c^2 + p_{ii}(\det P - p_{jj} T_{jj} - p_{ji} T_{ji}) c + p_{ii} p_{jj} T_{ji} - p_{ij} \det P = 0.$$

Thus deciding whether a 3×3 stochastic matrix can be embedded by 6 Poisson matrices amounts to at most checking 9 simple inequalities and solving 6 quadratic equations.

In general Poisson matrices of different types do not commute, i.e., A_{ij} and A_{lp} do not commute unless $(l,p) = (k,j)$. The following concept of extended commutativity is crucial for the development of Sect. 3 and seems to be relevant for the embedding problem in general.

Definition 1.1. We say that Poisson matrices A_{ij} and A_{lp} *commute in the extended sense* if for any $0<u_1, u_2<1$ there are constants $0<w_1, w_2<1$ such that

$$A_{ij}(u_1)A_{lp}(u_2)=A_{lp}(w_1)A_{ij}(w_2).$$

A_{ij} and A_{lp} commute in the extended sense if $(l,p)=(k,j)$, (i,k), or (j,i) (see Lemma 3.2). A_{ij} and A_{ki} do not commute even in the extended sense. However for any constants $0<u_1, u_2, u_3<1$ we can find constants $0<w_1$, $w_2, w_3<1$ such that

$$A_{ij}(u_1)\,A_{ki}(u_2)\,A_{ij}(u_3)=A_{ki}(w_1)\,A_{ij}(w_2)\,A_{ki}(w_3)$$

Similarly for A_{ij} and A_{jk} (see Lemma 3.5.).

In Sect. 3 we study the structure of the Bang-Bang representation for a 3×3 embeddable matrix $P>0$ with $B(P)<\det P$. Observe that the structure of the Bang-Bang representation for a matrix $P>0$ with $B(P)\geqq\det P>0$ is given in Theorem 1.2a).

The main theorem of Sect. 3 is that the *minimal Bang-Bang representation* for an embeddable 3×3 stochastic matrix $P>0$ with $B(P)<\det P$, i.e., the one that contains the smallest number of Poisson matrices among all possible Bang-Bang representations for P, has the following structure

$$P=(A_{ki}A_{jk}A_{ij}A_{ki}A_{jk})(A_{ij}A_{ki}A_{jk}A_{ij}\ldots) \quad \text{for some } (i,j,k)\in S \tag{1.6}$$

where the product of Poisson matrices in the first parenthesis is a positive stochastic matrix, say P', with the property $B'(j,i)=\det P'$.

Notice that the representation (1.6) consists of only 3 types of Poisson matrices that repeat in cycles of size 3. This is in contrast to the Bang-Bang representation for a matrix $P>0$ with $B(P)>\det P>0$ which consists in general of 5 or all 6 types of Poisson matrices, see Theorem 1.2a).

Johansen [6] showed that the number of Poisson matrices in the Bang-Bang representation for 3×3 embeddable matrix P is bounded by 6 times the smallest integer larger than or equal to $(ln\,\frac{1}{2})^{-1}\,ln\det P$.

This bound together with the knowledge of the structure of the minimal Bang-Bang representation for a 3×3 stochastic matrix $P>0$ with $B(P)<\det P$ allows in principle to determine whether a 3×3 stochastic matrix is embeddable or not. The algorithm is discussed in Sect. 3.

2. Sufficient and Necessary Condition for a Positive Matrix to be Embeddable by 6 Poisson Matrices

We first prove several lemmas. The first lemma is a special case of Theorem 1.1.

Lemma 2.1. *Let P be a matrix such that $p_{ik}=0$ for some $(i,j,k)\in S$. If $\prod_{i=1}^{3} p_{ii} =\det P>0$ then P is embeddable by 4 Poisson mattices in the following way: $P =A_{ki}A_{jk}A_{ij}A_{ki}$.*

Proof. Since ($p_{ik}=0$ and $p_{ii}p_{jj}p_{kk}=\det P$) $\Rightarrow$ ($T_{ij}<0$) the proof of this lemma is the same as the proof of Theorem 1.1 for the case $T_{ij}<0$, see [1]. Observe that equality $\prod_{i=1}^{3} p_{ii}=\det P$ implies that one needs 4 rather than 5 Poisson matrices to embed P.

Lemma 2.2 *Assume $P>0$ and for some $(i,j,k)\in S$ $B(i,i)\leqq \det P$ and $B(j,i)=\det P$. Then P is embeddable by 5 Poisson matrices as follows: $P=A_{ki}A_{jk}A_{ij}A_{ki}A_{jk}$.*

Proof. Assume $B(j,i)=\det P$ and let $P_1=PZ_{jk}\left(\frac{p_{ik}}{p_{ij}}\right)$. Then we have

$$p_{kk}^{(1)}=\frac{T_{ji}}{p_{ij}}, \qquad p_{ik}^{(1)}=0, \qquad p_{jk}^{(1)}=\frac{1}{p_{ij}}(-T_{ki})$$

and

$$p_{ii}^{(1)}p_{jj}^{(1)}p_{kk}^{(1)}=p_{ii}p_{jj}\left(1+\frac{p_{ik}}{p_{ij}}\right)\frac{T_{ji}}{p_{ij}}=\left(1+\frac{p_{ik}}{p_{ij}}\right)\det P=\det P_1$$

where the second equality follows by assumption.

Now $0<\det P=p_{ii}T_{ii}-p_{ki}T_{ki}-p_{ji}T_{ji}$ and $T_{ji}>0$ imply that $T_{ki}<0$ since if $T_{ki}\geqq 0$ then $p_{ii}T_{ii}>\det P$ contrary to the assumption. Hence $p_{jk}^{(1)}>0$. Thus by Lemma 2.1 $P_1=A_{ki}A_{jk}A_{ij}A_{ki}$ and hence $P=A_{ki}A_{jk}A_{ij}A_{ki}A_{jk}$, as we wished to show.

Lemma 2.3. *Suppose $P>0$, $\det P>0$ and $B(P)<\det P$. Let $P_1=PZ_{ij}(c)$ where $0<c<\bar{c}_{ij}$. Assume $\exists\,(i,j,k)\in S$ and $0<c<\bar{c}_{ij}$ such that $B_1(j,i)\geqq \det P_1$. Then there exists $0<c<\bar{c}_{ij}$ such that $B_1(j,i)=\det P_1$ and P can be embedded as follows: $P=A_{ki}A_{jk}A_{ij}A_{ki}A_{jk}A_{ij}$.*

Proof. Assume $B_1(j,i)=p_{ii}^{(1)}p_{jj}^{(1)}\dfrac{T_{ji}^{(1)}}{p_{ij}^{(1)}}>\det P_1$ for some $0<c<\bar{c}_{ij}$, that is

$$f(c)\equiv p_{ii}(p_{jj}-cp_{ji})\frac{T_{ji}-cT_{jj}}{p_{ij}-cp_{ii}}>\det P \qquad \text{for some } 0<c<\bar{c}_{ij}.$$

Then it follows by continuity of $f(c)$, $0<c<\bar{c}_{ij}$ and the assumption $f(0)<\det P$, that there exists $0<c<\bar{c}_{ij}$, say c^*, such that $f(c^*)=\det P$. Thus if we let $P_1=PZ_{ij}(c^*)$, then $B_1(j,i)=\det P_1$. But by Lemma 1.2a) $B_1(n,m)<\det P_1$ for $(n,m)\neq(j,i)$. Hence application of Lemma 2.2 to $P_1=PZ_{ij}(c^*)$ completes the proof.

Lemma 2.4. *Suppose $P=\prod_{i=1}^{n} A_i>0$, $B(k,j)\geqq \det P>0$ for some $(j,i,k)\in S$ and $B(n,m)<\det P$ for $(n,m)\neq(k,j)$. Then $P_1=PA_n^{-1}\geqq 0$ if and only if $A_n^{-1}=Z_{ki}\left(\frac{p_{ji}}{p_{jk}}\right)$.*

Proof. Assume $A_n^{-1}=Z_{ki}\left(\frac{p_{ji}}{p_{jk}}\right)$, then $p_{ji}^{(1)}=0$, $p_{ki}^{(1)}=\dfrac{1}{p_{jk}}(-T_{ij})$ and $p_{ii}^{(1)}=\dfrac{T_{kj}}{p_{jk}}$. By assumption $T_{kj}>0$ and $p_{jj}T_{jj}<\det P$, hence $\det P=p_{jj}T_{jj}-p_{kj}T_{kj}-p_{ij}T_{ij}<p_{jj}T_{jj}-p_{ij}T_{ij}$ implies $T_{ij}<0$, showing that $p_{ki}^{(1)}>0$ and thus $P_1\geqq 0$. Notice that the condition $B(k,j)\geqq \det P>0$ ensures $\prod_{i=1}^{3} p_{ii}^{(1)}\geqq \det P_1$.

Now assume $A_n^{-1} \neq Z_{ki}\left(\frac{p_{ji}}{p_{jk}}\right)$ but $P_1 \geqq 0$. Then the condition $B(n,m) < \det P$ for $(n,m) \neq (k,j)$ implies that $\prod_{i=1}^{3} p_{ii}^{(1)} < \det P_1$ which is impossible. This completes the proof.

Lemma 2.5. *Assume $P>0$, $B(k,j) \geqq \det P > 0$ for some $(i,j,k) \in S$ and $B(n,m) < \det P$ for $(n,m) \neq (k,j)$. Then at least 5 Poisson matrices are needed to embed P.*

Proof (by contradiction). Suppose $P = \prod_{m=1}^{4} A_m$, $B(k,j) \geqq \det P$, and let $P_1 = PA_4^{-1}$. Since 4 is the smallest number of Poisson matrices that can possibly embed a positive matrix we must have $P_1 \geqq 0$. Hence by Lemma 2.4 $P_1 = PZ_{ki}\left(\frac{p_{ji}}{p_{jk}}\right)$ and P_1 has only one element equal to zero, namely $p_{ji}^{(1)}$. Now observe that the only way P_1 can be embedded by 3 Poisson matrices is for $P_2 = P_1 A_3^{-1}$ to have 3 elements equal to zero and these elements in addition to $p_{ji}^{(2)} = 0$ have to be $p_{ik}^{(2)}$ and $p_{jk}^{(2)}$. We will now show that it is impossible to get $p_{ik}^{(2)} = p_{jk}^{(2)} = 0$ thus deriving the contradiction. In order to get $p_{ik}^{(2)} = p_{jk}^{(2)} = 0$ we must have $A_3^{-1} = Z_{jk}\left(\frac{p_{ik}^{(1)}}{p_{ij}^{(1)}}\right)$ or $A_3^{-1} = Z_{jk}\left(\frac{p_{jk}^{(1)}}{p_{jj}^{(1)}}\right)$. However, notice that if we let $P_2 = P_1 Z_{jk}\left(\frac{p_{jk}^{(1)}}{p_{jj}^{(1)}}\right)$, then

$$p_{ik}^{(2)} = p_{ik}^{(1)} - \frac{p_{jk}^{(1)}}{p_{jj}^{(1)}} p_{ij}^{(1)} = \frac{1}{p_{jj}^{(1)}} T_{ki}^{(1)} < 0$$

since $T_{kj} > 0$ and $B(k,k) < \det P$ imply that $T_{ki} < 0$ and hence $T_{ki}^{(1)} = \left(1 + \frac{p_{ji}}{p_{jk}}\right) T_{ki} < 0$. Now if $P_2 = P_1 Z_{jk}\left(\frac{p_{ik}^{(1)}}{p_{ij}^{(1)}}\right)$ then $p_{ik}^{(1)} = 0$, but

$$p_{jk}^{(2)} = p_{jk}^{(1)} - \frac{p_{ik}^{(1)}}{p_{ij}^{(1)}} p_{jj}^{(1)} = \frac{1}{p_{ij}^{(1)}} (-T_{ki}^{(1)}) > 0.$$

This completes the proof.

We can now prove

Theorem 2.1. *A necessary and sufficient condition for a positive matrix P to be embeddable by at most 6 Poisson matrices is*

$$B(i,j) \equiv p_{ii} p_{jj} \frac{T_{ij}}{p_{ji}} \geqq \det P > 0 \qquad \textit{for some } i,j = 1,2,3 \tag{2.1}$$

or that $\exists (i,j,k) \in S$ and $0 < c < \bar{c}_{ij}$ such that

$$B_1(j,i) = \det P_1 > 0 \qquad \textit{where } P_1 = PZ_{ij}(c). \tag{2.2}$$

Equation (2.2) is equivalent to the following quadratic equation in c

$$p_{ji} p_{ii} T_{jj} c^2 + p_{ii} (\det P - p_{jj} T_{jj} - p_{ji} T_{ji}) c + p_{ii} p_{jj} T_{ji} - p_{ij} \det P = 0.$$

Proof.

Sufficiency: If $B(P) \geqq \det P$ then $P = \prod_{m=1}^{6} A_m$ by Theorem 1.2a). Next suppose $B(P) < \det P$ and let $P_1 = PZ_{ij}(c) > 0$ be the matrix satisfying $B_1(j,i) = \det P_1$. By Lemma 1.2a) $B_1(n,m) < \det P_1$ for $(n,m) \neq (j,i)$ and hence by Lemma 2.2 P_1 is embeddable by 5 and P by 6 Poisson matrices.

Necessity (by contradiction). Let $P = \prod_{m=1}^{6} A_m$, $P_1 = PA_6^{-1}$ and suppose that P does not satisfy (2.1) or (2.2). Then by Lemma 1.1 $P_1 > 0$ and by Lemma 2.3 $B(P_1) < \det P_1$. Next, applying Lemma 1.1 to P_1 we get $0 < P_2 = \prod_{m=1}^{4} A_m$. Now since 4 is the smallest number of Poisson matrices that can possibly embed a positive matrix we must have $P_3 = \prod_{m=1}^{3} A_m \geqq 0$. Hence by Lemmas 1.1 and 1.2a) $B_2(k,j) \geqq \det P_2$ for some $(i,j,k) \in S$ and $B_2(n,m) < \det P_2$ for all $(n,m) \neq (k,j)$. But then by Lemma 2.5 at least 5 Poisson matrices are needed to embed P_2, contradicting $P_2 = \prod_{m=1}^{4} A_m$.

3. The Structure of 3×3 Embeddable Matrices

We will denote by $P_{(j,i)}$, $(i,j,k) \in S$, a positive matrix P which satisfies $B(j,i) = \det P > 0$ and $B(n,m) < \det P$ for $(n,m) \neq (j,i)$.

Lemma 3.1. *Suppose that $P > 0$ is an embeddable matrix but $B(P) < \det P$. Then P can be represented as*

$$P = P_{(j,i)} A_1 A_2 \dots A_n \quad \textit{for some } (i,j,k) \in S \textit{ and some Poisson matrices } A_1, A_2, \dots, A_n,\ n \geqq 1 \tag{3.1}$$

such that is we let $P_s = P_{(j,i)} A_1 A_2 \dots A_{n-s}$, $1 \leqq s \leqq n-1$ then $P_s > 0$ and

$$B(P_s) < \det P_s \quad \textit{for } 1 \leqq s \leqq n-1.$$

Proof. Immediate from Lemma 1.1 and Lemma 2.3.

The representation described in Lemma 3.1 is highly nonunique. First, there may be more than one permutation $(i,j,k) \in S$ for which P has representation (3.1). Two, for any $(i,j,k) \in S$ for which P has representation (3.1), there are many choices of the matrix $P_{(j,i)}$, the Poisson matrices $A_1, A_2, \dots, A_n$, and their number n such that $P = P_{(j,i)} A_1 A_2 \dots A_n$.

Let P be as in Lemma 3.1. Let $S_P \in S$ denote the set of permutations for which P has representation described in Lemma 3.1. For $(i,j,k) \in S_P$ let n_{ji} = smallest n, i.e., smallest number of Poisson matrices $A_1, A_2, \dots, A_n$, such that (3.1) holds. Consider the set R of representations for P.

$$R = \{P_{(j,i)} A_1 A_2 \dots A_{n_{ji}} \mid (i,j,k) \in S_p\}.$$

Let $\bar{n}=\min\{n_{ji}|(i,j,k)\in S_p\}$. We will call any representation in the set R for which $n_{ji}=\bar{n}$, a *minimal representation* for P and write it as $P_{(j,i)}A_1A_2\dots A_{\bar{n}}$. We will call $A_1A_2\dots A_{\bar{n}}$ a *minimal product* for P.

The structure of $P_{(j,i)}$ is given in Lemma 2.2. In order to investigate the structure of the minimal product for P, we introduce the concept of extended commutativity, see Definition 1.1.

The following definition is identical in nature to Definition 1.1.

Definition 3.1. We say that $Z_{ij}\equiv A_{ij}^{-1}$ and $Z_{lp}\equiv A_{lp}^{-1}$ commute in the extended sense if for any constants $c_1, c_2>0$ we can find constants $b_1, b_2>0$ such that

$$Z_{ij}(c_1)Z_{lp}(c_2)=Z_{lp}(b_1)Z_{ij}(b_2).$$

In all that follows the word "commute" is used in the extended sense.

Clearly, A_{ij} and A_{lp} commute if and only if Z_{ij} and Z_{lp} commute.

Lemma 3.2. *A_{ij} and A_{lp} commute if and only if $(l,p)=(k,j)$, (i,k), (j,i), (i,j).*

Proof. Clearly, $A_{ij}(u_1)A_{ij}(u_2)=A_{ij}(u_2)A_{ij}(u_1)=A_{ij}(u)$ where $u=u_1+u_2-u_1u_2$. A_{ij} and A_{kj} commute in the usual sense, i.e., for any $0<u_1, u_2<1$

$$A_{ij}(u_1)A_{kj}(u_2)=A_{kj}(u_2)A_{ij}(u_1).$$

Now it is easy to check that

$$A_{ij}(u_1)A_{ik}(u_2)=A_{ik}(w_1)A_{ij}(w_2)$$

if $w_1=(1-u_1)u_2$ and $w_2=\dfrac{u_1}{1-u_2+u_1u_2}$, while

$$A_{ij}(u_1)A_{ji}(u_2)=A_{ji}(w_1)A_{ij}(w_2)$$

if $w_1=\dfrac{u_2}{1-u_1+u_1u_2}$ and $w_2=u_1(1-u_2)$.

It is clear that A_{ij} and A_{lp} do not commute if $(l,p)=(j,k)$ or $(l,p)=(k,i)$. This completes the proof.

Lemma 3.3. *For any $0<u_1, u_2, u_3<1$ we can find $0<w_1, w_2, w_3<1$ such that*

$$A_{jk}(u_1)A_{ij}(u_2)A_{jk}(u_3)=A_{ij}(w_1)A_{jk}(w_2)A_{ij}(w_3) \tag{3.2}$$

Proof. It is a matter of simple computation to check that if we let

$$w_1=\frac{u_2u_3}{u_1+u_3-u_1u_3},\quad w_2=u_1+u_3-u_1u_3 \text{ and } w_3=\frac{u_1u_2(1-u_3)}{u_1(1-u_3)+u_3(1-u_2)}$$

then (3.2) holds. Clearly $0<w_1, w_2, w_3<1$.

Lemma 3.4. *Suppose $P>0$, $B(P)<\det P$ and let $P_{(j,i)}A_1A_2A_3\dots A_{\bar{n}}$, $n\geqq 1$ be a minimal representation for P. Then $A_1=A_{ij}$ and $A_2=A_{ki}$.*

Proof. If $\bar{n}=1$ then Lemma 1.2a) together with the definition of $P_{(j,i)}$ show that $A_1=A_{ij}$. Next suppose $\bar{n}=2$, that is $P=P_{(j,i)}A_1A_2$. Clearly $P_{(j,i)}A_1$ is then a minimal representation for PA_2^{-1} with $\bar{n}=1$. Hence $A_1=A_{ij}$. We will show that $A_2=A_{ki}$ by elimination of all other possibilities. If $A_2=A_{ik}$, A_{kj} or A_{ji} we have by Lemma 3.2

$$P=P_{(j,i)}A_{ij}(u_1)A_2(u_2)=P_{(j,i)}A_2(w_1)A_{ij}(w_2) \quad \text{for some } 0<w_1, w_2<1.$$

But then $P_{(j,i)}A_2(w_1)A_{ij}(w_2)$ is also a minimal representation for P which is impossible since $A_2 \neq A_{ij}$. Hence $A_2 \neq A_{ik}, A_{kj}, A_{ji}$ and it remains to be shown that $A_2 \neq A_{jk}$. Suppose to the contrary that

$$P=P_{(j,i)}A_{ij}(u_2)A_{jk}(u_1) \quad \text{for some } 0<u_1, u_2<1$$

let

$$P_2=PZ_{jk}(c_1)Z_{ij}(c_2) \quad \text{where } c_i=\frac{u_i}{1-u_i},\ i=1,2.$$

We will show directly that $B_2(j,i)<\det P_2$, thus contradicting $P_2=P_{(j,i)}$. We have

$$\begin{aligned} B_2(j,i)&=p_{jj}^{(2)}p_{ii}^{(2)}\frac{T_{ji}^{(2)}}{p_{ij}^{(2)}} \\ &=\frac{\left(p_{jj}-\frac{c_2}{1+c_1}p_{ji}\right)}{\left(p_{ij}-\frac{c_2}{1+c_1}p_{ii}\right)}p_{ii}\left[T_{ji}-\frac{c_2}{1+c_1}(T_{jj}-c_1T_{jk})\right](1+c_1)(1+c_2). \end{aligned} \tag{3.3}$$

If $B_2(j,i)\geqq \det P_2$ then clearly $T_{ji}^{(2)}>0$ and we must have $T_{jk}^{(2)}=(1+c_1)(1+c_2)T_{jk}<0$, and hence $T_{jk}<0$, since otherwise $\det P_2>0$ would imply that $p_{jj}^{(2)}T_{jj}^{(2)}>\det P_2$, which by Lemma 1.2a) is impossible. Hence letting $c=\frac{c_2}{1+c_1}$ in (3.3), using the fact that $T_{jk}<0$ and defining $P_1=PZ_{ij}(c)$ we get

$$\begin{aligned} \frac{B_2(j,i)}{(1+c_1)(1+c_2)}&=\frac{(p_{jj}-cp_{ji})}{(p_{ij}-cp_{ii})}p_{ii}[T_{ji}-cT_{jj}+c\cdot c_1T_{jk}] \\ &<\frac{(p_{jj}-cp_{ji})}{(p_{ij}-cp_{ii})}p_{ii}[T_{ji}-cT_{jj}]=\frac{B_1(j,i)}{1+c}. \end{aligned}$$

Now observe that $B_1(j,i)<\det P_1$ or equivalently $\frac{B_1(j,i)}{1+c}<\det P$ since otherwise the minimal product for P would consist of 1 rather than 2 Poisson matrices. Hence $B_2(j,i)<\det P_2$ as we wanted to show. This concludes the proof for $\bar{n}=2$.

If $P=P_{(j,i)}A_1A_2\ldots A_{\bar{n}}$, $\bar{n}>2$, is a minimal representation for P then $P_{(j,i)}A_1A_2$ is a minimal representation for $PA_{\bar{n}}^{-1}A_{\bar{n}-1}^{-1}\ldots A_3^{-1}$. Hence $A_1=A_{ij}$ and $A_2=A_{ki}$.

Theorem 3.1. *The minimal representation for an embeddable matrix $P>0$ such that $B(P)<\det P$ has the structure*

$$\begin{gathered} P=P_{(j,i)}(A_{ij}A_{ki}A_{jk}A_{ij}\ldots)=(A_{ki}A_{jk}A_{ij}A_{ki}A_{jk})(A_{ij}A_{ki}A_{jk}A_{ij}\ldots) \\ \textit{for some } (i,j,k)\in S \end{gathered} \tag{3.4}$$

where the product of Poisson matrices in the first parenthesis represents $P_{(j,i)}$ and the product in the second parenthesis is finite.

Proof (by induction on $\bar{n}$-size of the minimal product).

The representation of $P_{(j,i)}$ is given in Lemma 2.2. The theorem was proved for $\bar{n}=1$ and $\bar{n}=2$ in Lemma 3.4. Assume that the theorem is true for $\bar{n}=N$ and suppose that a minimal product in a minimal representation for P is of size $N+1$, i.e.

$$P=P_{(j,i)}A_1 A_2 \dots A_N, A_{N+1} \qquad \text{for some } (i,j,k)\in S.$$

Clearly $P_{(j,i)}A_1 A_2 \dots A_N$ is then a minimal representation for PA_{N+1}^{-1}, hence by induction assumption we have

$$A_1 A_2 \dots A_N A_{N+1} = \underbrace{A_{ij}A_{ki}A_{jk}A_{ij} \dots A_{ki}}_{N \text{ matrices}}A_{lp}$$

for some $(l,p,r)\in S$. We will show that $(l,p)=(j,k)$ by elimination of all other possibilities. Clearly $(l,p)\neq(k,i)$ since by assumption a minimal product for P consists of $N+1$ Poisson matrices. Suppose $(l,p)=(j,i)$, (k,j) or (i,k). Then applying Lemma 3.2 repeatedly we get

$$\begin{aligned} P&=P_{(j,i)}A_{ij}(u_1)\,A_{ki}(u_2)\,A_{jk}(u_3)\dots A_{ki}(u_N)\,A_{lp}(u_{N+1})\\ &=P_{(j,i)}\,A_{lp}(w_1)\,A_{ij}(w_2)\,A_{ki}(w_3)\,A_{jk}(w_4)\dots A_{ij}(w_N)\,A_{ki}(w_{N+1})\\ &\quad \text{for some } 0<w_1, w_2, \dots, w_{N+1}<1 \end{aligned}$$

which implies that there is a minimal representation for P with the first matrix in the minimal product different from A_{ij} which according to Lemma 3.4 is impossible. Hence $(l,p)\neq(j,i)$, (k,j), (i,k). Finally, suppose $(l,p)=(i,j)$, i.e.

$$\begin{aligned} P&=P_{(j,i)}A_{ij}(u_1)\,A_{ki}(u_2)\,A_{jk}(u_3)\dots A_{ij}(u_{N-1})\,A_{ki}(u_N)\,A_{ij}(u_{N+1})\\ &\quad \text{for some } 0<u_1, u_2, u_3, \dots, u_{N+1}<1. \end{aligned}$$

Then repeated application of Lemma 3.3 gives

$$\begin{aligned} P&=P_{(j,i)}\,A_{ki}(w_1)\,A_{ij}(w_2)\,A_{ki}(w_3)\dots A_{ij}(w_N)\,A_{ki}(w_{N+1})\\ &\quad \text{for some } 0<w_1, w_2, w_3, \dots, w_{N+1}<1 \quad \text{if } N \text{ is even} \end{aligned} \tag{3.5}$$

and

$$\begin{aligned} P&=P_{(j,i)}\,A_{ij}(u_1)\,A_{jk}(z_1)\,A_{ki}(z_2)\dots A_{ij}(z_{N-1})\,A_{ki}(z_N)\\ &\quad \text{for some } 0<z_1, z_2, \dots, z_N<1 \quad \text{if } N \text{ is odd.} \end{aligned} \tag{3.6}$$

Thus when N is even (3.5) is a minimal representation for P with the first matrix in the minimal product different from A_{ij}, while when N is odd (3.6) is a minimal representation for P with a second matrix in a minimal product different from A_{ki}, which is impossible by Lemma 3.4. This completes the proof.

Theorem 3.1 together with the bound on the number of Poisson matrices in the Bang-Bang representation, see introduction, suggest the following algorithm for determining whether a given 3×3 stochastic matrix is embeddable or not.

We start by asking whether a given matrix $P>0$, which is not embeddable by 6 Poisson matrices can be embedded by 7 Poisson matrices. Let $P_2 = PZ_{ij}(c_1) Z_{jk}(c_2) \equiv P_1 Z_{jk}(c_2)$. By (3.4) the question becomes: are there $(i,j,k) \in S$ and constants $0<c_1<\bar{c}_{ij}$, $0<c_2<\bar{c}_{jk}^{(1)}$ such that $B_2(k,j)=\det P_2$. If the answer is negative we ask about embeddability of P by 8 Poisson matrices. Let

$$P_3 = PZ_{ij}(c_1) Z_{jk}(c_2) Z_{ki}(c_3) \equiv P_1 Z_{jk}(c_2) Z_{ki}(c_3) \equiv P_2 Z_{ki}(c_3)$$

and ask are there $(i,j,k) \in S$ and constants $0<c_1<\bar{c}_{ij}$, $0<c_2<\bar{c}_{jk}^{(1)}$, $0<c_3<\bar{c}_{ki}^{(2)}$ such that $B_3(i,k)=\det P_3$. We continue this way until we find the right number of Poisson matrices that embed a given matrix or reach one plus the upper bound, whichever is smaller. In the last case we conclude that the matrix is not embeddable.

References

1. Frydman, H.: The Embedding Problem for Markov Chains with 3 States. Math. Proc. Cambridge Philos. Soc. **87**, 285–294 (1980)
2. Frydman, H., Singer, B.: Total Positivity and the Embedding Problem for Markov Chains. Math. Proc. Cambridge Philos. Soc. **86**, 339–344 (1979)
3. Goodman, G.S.: An Intrinsic Time for Nonstationary Finite Markov Chains. Z. Wahrscheinlichkeitstheorie verw. Gebiete **16**, 165–180 (1970)
4. Johansen, S.: A Central Limit Theorem for Finite Semigroups and Its Applications to the Imbedding Problem for Finite State Markov Chains. Z. Wahrscheinlichkeitstheorie verw. Gebiete **26**, 171–190 (1973)
5. Johansen, S.: The Bang-Bang Problem for Stochastic Matrices. Z. Wahrscheinlichkeitstheorie verw. Gebiete **26**, 191–195 (1973)
6. Johansen, S., Ramsey, F.L.: A Bang-Bang Representation for 3×3 Imbeddable Stochastic Matrices. Z. Wahrscheinlichkeitstheorie verw. Gebiete **47**, 107–118 (1979)
7. Kingman, J.F.C., Williams, David: A Combinatorial Structure of Nonhomogeneous Markov Chains. Z. Wahrscheinlichkeitstheorie verw. Gebiete **26**, 77–86 (1973)
8. Lee, E.B., Marcus, L.: Foundations of Optimal Control. New York: Wiley 1968

Received October 25, 1979