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The embedding problem for Markov chains with three states

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1. *Introduction.* In this paper we consider the embedding problem for Markov chains with three states. A non-singular stochastic matrix P is called embeddable if there exists a two-parameter family of stochastic matrices

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

satisfying
$$P(s,t) = P(s,u)\,P(u,t), \quad 0 \leqslant s \leqslant u \leqslant t,$$
$$\lim_{t \downarrow s} P(s,t) = \lim_{s \uparrow t} P(s,t) = I$$

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

Though extensive characterizations of embeddable $n \times n$ stochastic matrices have been given in (1), (2), (3), (6), and further characterizations of embeddable 3×3 stochastic matrices in (4), they do not provide, except in the case of 2×2 stochastic matrices, easily applicable necessary and sufficient conditions for embeddability.†

The main purpose of this paper is to provide such conditions for certain classes of 3×3 stochastic matrices.

We use different methods than those employed in (4) and (5) and, as a by-product of our investigation, obtain a new algebraic proof of Bang–Bang representation for 3×3 embeddable stochastic matrices.

For our development we will require the following general characterization of embeddable matrices formulated by Johansen (2):

(A) A non-singular stochastic matrix P is embeddable iff it can be approximated by a finite product of Poisson matrices;

and the necessary condition for embeddability of stochastic matrices due to Goodman (1):

(B) If $P = \|p_{ij}\|$ is an embeddable $n \times n$ stochastic matrix then

$$\prod_{i=1}^{n} p_{ii} \geqslant \det P > 0.$$

It was conjectured by Goodman in (1) that (B) is also a sufficient condition for a stochastic matrix P to be embeddable. However Kingman and Williams (6) constructed a counterexample using 4×4 matrices based on their analysis of allowable patterns of zeros in embeddable matrices.

† After this paper was written it was brought to my attention that some of the conditions I have found were also obtained by Johansen & Ramsey in (5), their new version of (4). See also (7) for the complete solution to the embedding problem for the class of birth and death processes.

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The starting point for this work was the observation that for 3×3 stochastic matrices a counterexample to Goodman's conjecture analogous to that of Kingman and Williams cannot be constructed. Thus, in § 3 we prove that

$$\prod_{i=1}^{3} p_{ii} \geqslant \det P > 0$$

is a sufficient condition for embeddability of a 3×3 stochastic matrix with at least one off-diagonal element equal to zero, and in this case

$$P = \prod_{m=1}^{5} A_m,$$

where A_m, $1 \leqslant m \leqslant 5$, are Poisson matrices.

The remainder of the paper is concerned with the question of embeddability of positive (all elements positive) 3×3 stochastic matrices and the following observation is basic for its development. Let P be a positive 3×3 stochastic matrix and P^* an embeddable 3×3 stochastic matrix with one off-diagonal element equal to 0. If P and P^* are related as follows

$$P^* = PA^{-1},$$

where A is a Poisson matrix, then P must satisfy

$$B(n,m) \equiv p_{nn}p_{mm}\frac{T_{nm}}{p_{mn}} \geqslant \det P \quad \text{for some } (n,m), \quad n,m = 1,2,3,$$

where

$$T_{nm} = M_{nm}(-1)^{n+m-1} \quad \text{for} \quad n \neq m,$$
$$T_{nn} = M_{nn}$$

and M_{nm}, M_{nn} denote second-order minors of P.

In § 4 we prove that the condition $\max_{(n,m)} B(n,m) \geqslant \det P > 0$ is sufficient for embeddability of a positive matrix and in this case matrix P can be embedded by 6 Poisson matrices. We also obtain the characterization of regular matrices (i.e. matrices with positive principal minors) which can be embedded by 6 Poisson matrices. We conclude § 4 by giving a sufficient condition for a positive matrix P, for which

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

to be embeddable by 7 Poisson matrices.

In § 5 we prove that the condition $\max_{(n,m)} B(n,m) \geqslant \det P > 0$ is necessary for embeddability of a matrix P with $\det P \geqslant \frac{1}{2}$. From this result the proof of Bang–Bang representation easily follows.

2. *Preliminaries.* 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 $P \geqslant 0$ a matrix with at least one off-diagonal element equal to zero and the remaining elements positive.

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Let $S = \{(i,j,k) | (i,j,k)$ be a permutation of $(1,2,3)\}$ and let M_{ij}, M_{ii} denote second-order minors of P, i.e.

$$M_{ij} = (p_{ji}\,p_{kk} - p_{jk}\,p_{ki})\,(-1)^{i+j-1}$$
$$M_{ii} = (p_{jj}\,p_{kk} - p_{jk}\,p_{kj}) \quad (i,j,k) \in S.$$

Then define

$$\left.\begin{aligned} T_{ij} &= M_{ij}(-1)^{i+j-1}, \\ T_{ii} &= M_{ii} \end{aligned}\right\} \tag{2·1}$$

and observe that for every $(i,j,k) \in S$

$$\det P = p_{kk}T_{kk} - p_{jk}T_{jk} - p_{ik}T_{ik} = p_{jj}T_{jj} - p_{jk}T_{jk} - p_{ji}T_{ji}. \tag{2·2}$$

Let E_{ij} be a matrix with elements

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

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

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

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

$$Z_{ij}(c) = I + cE_{ii} - cE_{ij}, \quad c = \frac{u}{1-u} \geqslant 0. \tag{2·3}$$

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

$$p_r^* = \begin{cases} p_r & \text{if} \quad r \neq i,j \\ p_j - cp_i & \text{if} \quad r = j \\ p_i(1+c) & \text{if} \quad r = i \end{cases} \tag{2·4}$$

and

$$\det P^* = (1+c)\det P.$$

Note that $P^* = \|p_{ij}^*\|$ satisfies $\sum_{j=1}^{3} p_{ij}^* = 1;\ 1 \leqslant i \leqslant 3$ but may not be stochastic.

3. *Embeddability of a matrix with at least one off-diagonal element equal to* 0

THEOREM 3·1. *Let P be a matrix with $\det P > 0$ and such that $p_{ij} = 0$ for some $(i \neq j)$. Then the following are equivalent*

(i) *P is embeddable,*

(ii) $\prod_{i=1}^{3} p_{ii} \geqslant \det P$,

(iii) $P = \prod_{m=1}^{5} A_m$ *where $(A_m, 1 \leqslant m \leqslant 5)$ are Poisson matrices.*

It is known that (iii) ⇒ (i) ⇒ (ii). It remains to show that (ii) ⇒ (iii).

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

$$T_{ij}^{(m)} = p_{ji}^{(m)}p_{kk}^{(m)} - p_{jk}^{(m)}p_{ki}^{(m)} \quad \text{and} \quad P_0 \equiv P.$$

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Outline of the proof. We prove that (ii) → (iii) by explicit construction of

$$(A_m,\ 1 \leqslant m \leqslant 5).$$

The method of construction is as follows:

At the mth step ($1 \leqslant m \leqslant 5$) we use one of the inequalities

$$\prod_{i=1}^{3} p_{ii}^{(m-1)} \geqslant \det P_{m-1}, \quad \det P_{m-1} > 0$$

– provided that both inequalities are not automatically satisfied as a consequence of the pattern of zeros in the matrix P_{m-1} – to show that we can construct a Poisson matrix, say A, such that

(1) $P_m = P_{m-1}A^{-1}$ has one more zero element than P_{m-1},

(2) $P_m \geqslant 0$,

(3) $\prod_{i=1}^{3} p_{ii}^{(m)} \geqslant \det P_m$.

If both inequalities are automatically satisfied we use the pattern of zeros in P_{m-1} to show that we can construct A so that (1) and (2) hold. Note that at the first step we construct the matrix A_5, at the second step the matrix A_4, and so on.

Proof. Let $p_{ij} = 0$ for some $(i,j,k) \in S$. Then condition $p_{ii}\,p_{jj}\,p_{kk} \geqslant \det P$ can be written using (2·2) as

$$p_{ik}T_{ik} + p_{ii}\,p_{kj}\,p_{jk} \geqslant 0.$$

We will first consider the case when $T_{ik} \geqslant 0$. Let $P_1 = PZ_{ji}\left(\frac{p_{ji}}{p_{jj}}\right)$. Then by (2·4)

$$p_{nm}^{(1)} = 0 \quad \text{for} \quad (n,m) = (j,i), (i,j) \quad \text{and, since} \quad T_{ik} \geqslant 0, \quad P_1 \geqslant 0.$$

Now let $P_2 = P_1 Z_{ik}\left(\frac{p_{ik}^{(1)}}{p_{ii}^{(1)}}\right)$. Then $p_{nm}^{(2)} = 0$ for $(n,m) = (j,i),\ (i,j), (i,k)$ and since $\det P_1 = p_{jj}^{(1)}T_{jj}^{(1)} - p_{jk}^{(1)}p_{kj}^{(1)}p_{ii}^{(1)} > 0$ implies $T_{jj}^{(1)} > 0$ we have $P_2 \geqslant 0$.

Next let $P_3 = P_2 Z_{kj}\left(\frac{p_{kj}^{(2)}}{p_{kk}^{(2)}}\right)$. Then $p_{nm}^{(3)} = 0$ for $(n \neq m) \neq (k,i), (j,k)$ and since $\det P_2 = T_{ii}^{(2)} > 0$ we have $P_3 \geqslant 0$.

Let $P_4 = P_3 Z_{jk}\left(\frac{p_{jk}^{(3)}}{p_{jj}^{(3)}}\right)$. Then $p_{nm}^{(4)} = 0$ for $(n \neq m) \neq (k,i)$ and clearly $P_4 \geqslant 0$.

Finally, let $P_5 = P_4 Z_{ki}\left(\frac{p_{ki}^{(4)}}{p_{kk}^{(4)}}\right)$. Then $P_5 = I$, and hence P can be represented as the following product of Poisson matrices

$$P = A_{ki}\left(\frac{p_{ki}^{(4)}}{p_{kk}^{(4)} + p_{ki}^{(4)}}\right) A_{jk}\left(\frac{p_{jk}^{(3)}}{p_{jj}^{(3)} + p_{jk}^{(3)}}\right) A_{kj}\left(\frac{p_{kj}^{(2)}}{p_{kk}^{(2)} + p_{kj}^{(2)}}\right) A_{ik}\left(\frac{p_{ik}^{(1)}}{p_{ii}^{(1)} + p_{ik}^{(1)}}\right) A_{ji}\left(\frac{p_{ji}}{p_{jj} + p_{ji}}\right).$$

If $T_{ik} < 0$ let $P_1 = PZ_{ji}\left(\frac{p_{ki}}{p_{kj}}\right)$. Then $p_{nm}^{(1)} = 0$ for $(n,m) = (i,j), (k,i)$ and, since

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$T_{ik} < 0$, $P_1 \geqslant 0$. Also observe that

$$p_{ii}^{(1)} p_{jj}^{(1)} p_{kk}^{(1)} = p_{jj}\left(1+\frac{p_{ki}}{p_{kj}}\right) p_{ii}\, p_{kk} \geqslant \det P \left(1+\frac{p_{ki}}{p_{kj}}\right) = \det P_1,$$

which is equivalent to

$$p_{kj}^{(1)} T_{kj}^{(1)} \geqslant \det P_1. \tag{3·1}$$

Now let $P_2 = P_1 Z_{ik}\left(\frac{p_{ik}^{(1)}}{p_{ii}^{(1)}}\right)$. Then $p_{nm}^{(1)} = 0$ for $(n,m) = (i,j), (k,i), (i,k)$ and since by inequality (3·1) $T_{kj}^{(1)} > 0$ we have $P_2 \geqslant 0$.

Next let $P_3 = P_2 Z_{kj}\left(\frac{p_{kj}^{(2)}}{p_{kk}^{(2)}}\right)$. Then $p_{nm}^{(3)} = 0$ for $(n \neq m) \neq (j,i), (j,k)$ and since $\det P_2 = T_{ii}^{(2)} > 0$ we have $P_3 \geqslant 0$.

Let $P_4 = P_3 Z_{jk}\left(\frac{p_{jk}^{(3)}}{p_{jj}^{(3)}}\right)$. Then $p_{nm}^{(4)} = 0$ for $(n \neq m) \neq (j,i)$ and clearly $P_4 \geqslant 0$.

Finally, let $P_5 = P_4 Z_{ji}\left(\frac{p_{ji}^{(4)}}{p_{jj}^{(4)}}\right)$. Then $P_5 = I$ and hence P can be embedded in the following way

$$P = A_{ji}\left(\frac{p_{ji}^{(4)}}{p_{jj}^{(4)}+p_{ji}^{(4)}}\right) A_{jk}\left(\frac{p_{jk}^{(3)}}{p_{jj}^{(3)}+p_{jk}^{(3)}}\right) A_{kj}\left(\frac{p_{kj}^{(2)}}{p_{kk}^{(2)}+p_{kj}^{(2)}}\right) A_{ik}\left(\frac{p_{ik}^{(1)}}{p_{ii}^{(1)}+p_{ik}^{(1)}}\right) A_{ji}\left(\frac{p_{ki}}{p_{kj}+p_{ki}}\right).$$

4. *Characterization of positive matrices that can be embedded by six Poisson matrices.* We will call a matrix P *regular* if all its principal minors are positive, i.e. if $T_{ii} > 0$ for all $1 \leqslant i \leqslant 3$.

For a positive matrix let

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

and

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

The following lemma shows the significance of the function $B(n,m)$ for the embedding problem.

LEMMA 4·1. *Let* $P = \prod_{m=1}^{l} A_m > 0$, *where* A_m, $1 \leqslant m \leqslant l$, *are Poisson matrices, and assume that* $\max_{(n,m)} B(n,m) < \det P$. *Then also* $PA_l^{-1} > 0$.

Proof. Let $P^* = PA_l^{-1} \equiv PZ_{ij}(c)$ for some $(i,j,k) \in S$. Clearly we must have $0 < c \leqslant \bar{c}_{ij}$, since otherwise at least one element of P^* is negative, contradicting the assumption about P^*. Now the only way we can have $P^* \geqslant 0$ rather than $P^* > 0$ is when $c = \bar{c}_{ij}$, that is, if $c = \frac{p_{ij}}{p_{ii}}$ or $c = \frac{p_{kj}}{p_{ki}}$ or $c = \frac{p_{jj}}{p_{ji}}$. But then in all three cases, as can be easily computed using $\max_{(n,m)} B(n,m) < \det P$, $\prod_{i=1}^{3} p_{ii}^{*} < \det P^*$, which is impossible since P^* is embeddable by assumption.

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The main result of this section is

THEOREM 4·1. *Let P be a positive matrix with* $\det P > 0$.

(*a*) *If* $\max_{(n,m)} B(n,m) \geqslant \det P$ *then P is embeddable and* $P = \prod_{m=1}^{6} A_m$.

(*b*) *If* $P = \prod_{m=1}^{6} A_m$ *and P is regular then* $\max_{(n,m)} B(n,m) \geqslant \det P$.

The proof of Theorem 4·1, which essentially depends on the analysis of different possible configurations of signs of minors of P, will follow after we prove two lemmas.

In the first lemma we consider the class of matrices for which condition

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

is automatically satisfied as a result of signs of minors of P. Let

$$E = \{P > 0 \mid \det P > 0, \text{ and for some } (i,j,k) \in S \ (T_{jk} \geqslant 0 \text{ and } T_{ik} \geqslant 0) \text{ or } (T_{ik} \geqslant 0 \text{ and } T_{ji} \geqslant 0)\}.$$

LEMMA 4·2. *If* $P \in E$ *then* $P = \prod_{m=1}^{6} A_m$ *and* $\max_{(n,m)} B(n,m) \geqslant \det P$.

Proof. Case 1: $T_{jk} \geqslant 0$ and $T_{ik} \geqslant 0$ for some $(i,j,k) \in S$. It follows from the inequality

$$\det P = p_{kk} T_{kk} - p_{ik} T_{ik} - p_{jk} T_{ik} > 0$$

that

$$p_{kk} T_{kk} \geqslant \det P. \tag{4·1}$$

Let

$$P^* = P Z_{ji}\left(\frac{p_{ji}}{p_{jj}}\right).$$

Then $p^*_{ji} = 0$ and since $T_{kk} > 0$ and $T_{ik} \geqslant 0$ we have $P^* \geqslant 0$. By (4·1)

$$p^*_{ii}\, p^*_{jj}\, p^*_{kk} = \left(p_{ii} - \frac{p_{ji}}{p_{jj}} p_{ij}\right) p_{jj} \left(1 + \frac{p_{ji}}{p_{jj}}\right) p_{kk} = p_{kk} T_{kk} \left(1 + \frac{p_{ji}}{p_{jj}}\right) \geqslant \det P^*.$$

Thus P^* satisfies all assumptions of Theorem 3·1 and so is embeddable by 5 Poisson matrices, but then P is embeddable by 6.

Case 2: $T_{jk} \geqslant 0$ and $T_{ji} \geqslant 0$ for some $(i,j,k) \in S$. We also assume that $T_{ik} < 0$ since otherwise we are in case 1. Let

$$P^* = P Z_{ji}\left(\frac{p_{ki}}{p_{kj}}\right).$$

Then $p^*_{ki} = 0$ and since $T_{jk} \geqslant 0$ and $T_{ik} < 0$, $P^* \geqslant 0$. Finally, observe that

$$T_{jk}\, p_{kk}\, p_{jj} - p_{kj} \det P = -T_{ik} T_{ji} + p_{jk}\, p_{kj} T_{jk} \geqslant 0,$$

which shows that $B(j,k) \geqslant \det P$, and therefore

$$p^*_{ii}\, p^*_{jj}\, p^*_{kk} = \frac{T_{jk}}{p_{kj}} p_{kk} p_{jj} \left(1 + \frac{p_{ki}}{p_{kj}}\right) \geqslant \det P^*.$$

Hence we can apply Theorem 3·1 to P^*, which completes proof of the lemma.

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LEMMA 4·3. *Let* $P > 0$ *be a matrix with* $\det P > 0$ *and such that* $\max B(n,m) < \det P$. *Let* $P^* = PZ_{ij}(c)$, *where* $(i,j,k) \in S$ *and* $0 < c < \bar{c}_{ij}$ *so that* $P^* > 0$. *Then*

(*a*) $$B^*(n,m) = p^*_{nn}p^*_{mm}\frac{T^*_{nm}}{p^*_{mn}} < \det P^* \quad \text{for all } (n,m) \neq (j,i), \tag{4·2}$$

(*b*) *If* P *is regular,* $B^*(n,m) < \det P^*$ *for all* (n,m).

Proof. (*a*) We will prove (4·2) by showing that if $B^*(n,m) > 0$ then for

$$(n,m) \neq (j,i),(i,i)$$

$$B^*(n,m) \leqslant (1+c)\,B(n,m) \tag{4·3}$$

while $$B^*(i,i) \leqslant \begin{cases} (1+c)\,B(i,i) & \text{if} \quad T_{ij} \geqslant 0 \\ B^*(i,k) & \text{if} \quad T_{ij} < 0. \end{cases}$$

It is an easy computation to check (4·3) for $(n,m) = (k,j), (i,k), (i,j), (k,k)$ and (j,j). Now consider $(n,m) = (j,k)$.

$$B^*(j,k) = (1+c)\,p_{kk}\frac{(p_{jj}-cp_{ji})}{(p_{kj}-cp_{ki})}T_{jk}.$$

Since $P \notin E$, $T_{jk} > 0$ implies $T_{ik} < 0$. But

$$(T_{ik} < 0) \Leftrightarrow \left(\frac{p_{jj}-cp_{ji}}{p_{kj}-cp_{ki}} < \frac{p_{jj}}{p_{kj}}\right).$$

Hence $$B^*(j,k) < (1+c)\,B(j,k).$$

In order to prove inequality (4·3) for $(n,m) = (k,i)$ we need the following result

$$(T_{ki} \leqslant 0) \Rightarrow (T^*_{ki} < 0). \tag{4·4}$$

Now $T^*_{ki} = T_{ki} + cT_{kj}$ and the case which requires proof is $T_{kj} > 0$. Consider the following inequality which holds by assumption

$$\det P - B(k,j) = p_{kk}T_{kk} - p_{ki}T_{ki} - p_{kj}T_{kj} - B(k,j) > 0. \tag{4·5}$$

But $$p_{kk}T_{kk} - B(k,j) = \frac{p_{kk}}{p_{jk}}p_{ji}T_{ki} \leqslant 0.$$

Hence in order for inequality (4·5) to hold we must have

$$T_{ki} + \frac{p_{kj}}{p_{ki}}T_{kj} < 0,$$

which together with $c < \dfrac{p_{kj}}{p_{ki}}$ shows that $T^*_{ki} < 0$. Hence (4.4) holds.

Now $$B^*(k,i) = (1+c)\frac{p_{kk}p_{ii}(T_{ki}+cT_{kj})}{p_{ik}}.$$

By (4·4) $T^*_{ki} > 0$ implies $T_{ki} > 0$ and therefore, since $P \notin E$, $T_{kj} < 0$. Hence

$$B^*(k,i) < (1+c)\,B(k,i).$$

Finally consider

$$B^*(i,i) = p_{ii}(1+c)\,(T_{ii} - cT_{ij}).$$

If $T_{ij} \geqslant 0$, then $B^*(i,i) \leqslant (1+c)\,B(i,i)$. If $T_{ij} < 0$, then $T^*_{ij} = (1+c)\,T_{ij} < 0$. But $(T^*_{ij} < 0) \Leftrightarrow [B^*(i,i) < B^*(i,k)]$. This completes the proof of part (*a*).

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(*b*) It remains to show that if P is regular then also $B^*(j,i) < \det P^*$. Assume $T^*_{ji} > 0$.

We will show that

$$B^*(j,i) \leqslant \begin{cases} (1+c)\,B(i,k) & \text{if} \quad D < 0 \\ (1+c)\,B(j,i) & \text{if} \quad D \geqslant 0, \end{cases}$$

where $$D \equiv p_{kk}\,p_{ji}\,p_{ij} - p_{jj}\,p_{ik}\,p_{ki}.$$

Now inequality $B^*(j,i) \leqslant (1+c)\,B(i,k)$ is equivalent to the inequality $D \leqslant c p_{ji} T_{jj}$, which is true if $D < 0$, since P is regular.

Inequality $B^*(j,i) \leqslant (1+c)\,B(j,i)$ can be rewritten as

$$p_{ij}\,D + p_{ik}\,p_{kj}\,T_{kk} \geqslant c p_{ji}\,p_{ij}\,T_{jj}$$

and observe that even if we replace c by its upper bound, i.e. $\dfrac{p_{kj}}{p_{ki}}$, we obtain

$$D(-T_{jk}) \geqslant 0,$$

a true inequality if $D > 0$ since $T_{jk} < 0$. That $T_{jk} < 0$ can be seen as follows:

$$T^*_{ji} = T_{ji} - c T_{jj} > 0$$

implies $T_{ji} > 0$, which, since $P \notin E$, implies in turn $T_{jk} < 0$. Hence

$$\max_{(n,m)} B^*(n,m) < \det P^*$$

and this completes the proof of Lemma 4·3.

COROLLARY 4·1. *Assume* $\det P > 0$, $\max B(n,m) < \det P$ *and let* $P^* = P Z_{ij}(c)$, $0 < c < \bar{c}_{ij}$. *If* $T_{jj} > 0$ *then* $\max\limits_{(n,m)} B^*(n,m) < \det P^*$.

Proof. See proof of Lemma 4·3.

Proof of Theorem 4·1. (*a*) Assume $\max\limits_{(n,m)} B(n,m) \geqslant \det P$. If $P \in E$ then $P = \prod\limits_{m=1}^{6} A_m$ by Lemma 4·2. Now observe that, for every $(i,j,k) \in S$, $[B(i,i) < B(i,j)] \Leftrightarrow [T_{ik} < 0]$ and $[B(i,i) < B(i,k)] \Leftrightarrow [T_{ij} < 0]$. Therefore if $P \notin E$ either $B(i,i) < B(i,j)$ or $B(i,i) < B(i,k)$. Hence in this case we may assume that $B(i,j) \geqslant \det P$ for some $i \neq j$. Then let $P^* = P Z_{ik}\left(\dfrac{p_{jk}}{p_{ji}}\right)$ and proceed as in case 2 of Lemma 4·2 (permuting $i \to k \to j \to i$).

(*b*) (By contradiction.) Assume P is regular, $P = \prod\limits_{m=1}^{6} A_m$, $\max\limits_{(n,m)} B(n,m) < \det P$. Let $P^* = P A_6^{-1}$ and $P^{**} = P^* A_5^{-1} = \prod\limits_{m=1}^{4} A_m$. By Lemma 4·1 $P^* > 0$ and by Lemma 4·3(*b*) $\max\limits_{(n,m)} B^*(n,m) < \det P^*$. If P^* is regular then again by Lemma 4·3(*b*)

$$\max_{(n,m)} B^{**}(n,m) < \det P^{**}$$

and so, by Lemma 4·1, $0 < P^{**} A_4^{-1} = A_1 A_2 A_3$, which is impossible since 4 is the smallest number of Poisson matrices that can possibly embed a positive matrix. Therefore P^* is not regular. We will next show that, even if P^* is not regular,

$$\max B^{**}(n,m) < \det P^{**}.$$

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Now, since $P^* = PZ_{ij}(c_1)$, $0 < c_1 < \bar{c}_{ij}$ is not regular, and since $T^*_{jj} = (1+c_1)T_{jj} > 0$ and $T^*_{kk} = (1+c_1)T_{kk} > 0$ we must have $T^*_{ii} = T_{ii} - c_1 T_{ij} \leqslant 0$ which implies that $T_{ij} > 0$. Hence by Corollary 4·1 if P^{**} is to satisfy $\max\limits_{(n,m)} B^{**}(n,m) \geqslant \det P^{**}$, we must have $P^{**} = P^*Z_{ki}(c_2)$, $0 < c_2 < \bar{c}^*_{ki}$ or $P^{**} = P^*Z_{ji}(c_2)$, $0 < c_2 < \bar{c}^*_{ji}$. If $P^{**} = P^*Z_{ki}(c_2)$ satisfies $\max\limits_{(n,m)} B^{**}(n,m) \geqslant \det P^{**}$ then by Lemma 4·3(*a*) $B^{**}(i,k) \geqslant \det P^{**}$, which implies $T^{**}_{ik} > 0$. But $T^{**}_{ik} > 0$ and $T^{**}_{ij} = (1+c_1)(1+c_2)T_{ij} > 0$ imply, since

$$\det P^{**} > 0,$$

that $T^{**}_{ii} = T^*_{ii}(1+c_2) > 0$, which is impossible since as we argued $T^*_{ii} \leqslant 0$. Thus in this case $\max\limits_{(n,m)} B^{**}(n,m) < \det P^{**}$.

If $P^{**} = PZ_{ij}(c_1)Z_{ji}(c_2)$ satisfies $\max\limits_{(n,m)} B^{**}(n,m) \geqslant \det P^{**}$ then by Lemma 4·3(*a*) $B^{**}(i,j) \geqslant \det P^{**}$. Now let $b_1 = c_2/(1+c_1+c_1c_2)$ and $b_2 = c_1(1+c_2)$. Then it is easy to check that $P^{**} = PZ_{ji}(b_1)Z_{ij}(b_2)$. But then applying Lemma 4·3(*a*) we get $B^{**}(i,j) < \det P^{**}$. This contradiction shows that $\max\limits_{(n,m)} B^{**}(n,m) < P^{**}$. But then, as we argued above, $P \neq \prod\limits_{m=1}^{6} A_m$, which contradicts the assumption.

Now suppose that P is a matrix with $\det P > 0$ but $\max\limits_{(n,m)} B(n,m) < \det P$, and consider $P^* = PZ_{ij}(c)$, $0 < c < \bar{c}_{ij}$. If $\max\limits_{(n,m)} B^*(n,m) \geqslant \det P^*$ then P^* can be embedded by 6 and hence P by 7 Poisson matrices. The following corollary tells how to check whether $\max B^*(n,m) \geqslant \det P^*$ for some $(i,j,k) \in S$ and $0 < c < \bar{c}_{ij}$.

COROLLARY 4·2 (*Sufficient condition for a non-regular matrix to be embeddable by 7 Poisson matrices.*)

Assume $\det P > 0$ and $\max\limits_{(n,m)} B(n,m) < \det P$. Let $P^* = PZ_{ij}(c)$, $0 < c < \bar{c}_{ij}$. Then P is embeddable by 7 Poisson matrices if $\exists\,(i,j,k) \in S$ and $0 < c < \bar{c}_{ij}$ such that

$$B^*(j,i) \geqslant \det P^*. \tag{4·6}$$

Inequality (4·6) represents the following quadratic inequality in c.

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

Also note that by Corollary 4·1 inequality (4·6) may hold only if $T_{jj} < 0$.

Proof. Immediate from Theorem 4·1.

5. *Embeddability of a matrix P with $\det P \geqslant \frac{1}{2}$ and a Bang–Bang representation.* Let

$$M = \{P > 0 | \det P \geqslant \tfrac{1}{2}\}.$$

THEOREM 5·1. *If $P \in M$ then P is embeddable if and only if* $\max\limits_{(n,m)} B(n,m) \geqslant \det P$.

Proof. If $\max\limits_{(n,m)} B(n,m) \geqslant \det P$ then P is embeddable by Theorem 4·1(*a*). We will prove the reverse implication by contradiction as follows.

Assume first that P can be represented as a finite product of Poisson matrices, i.e. $P = \prod\limits_{m=1}^{l} A_m$ but $\max\limits_{(n,m)} B(n,m) < \det P$, and consider $P^* = PZ_{ij}(c) = \prod\limits_{m=1}^{l-1} A_m$, where

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$Z_{ij}(c) \equiv A_l^{-1}$. Clearly, $\det P^* \geqslant \frac{1}{2}$, which implies that P^* is regular. By Lemma 4·1 $P^* > 0$. Hence we can apply lemma 4·3(*b*) and get that $\max B^*(n,m) < \det P^*$, thus showing that P^* is 'the same matrix as P'. Repeating this argument l times we obtain $P \prod_{m=0}^{l-1} A_{l-m}^{-1} > 0$. Contradiction.

Next assume that $P = \lim_{k\to\infty} P_k$, where $P_k = \prod_{i=1}^{N_k} A_{i,k}$, $k \geqslant 1$, and $A_{i,k}$ are Poisson matrices. Then we can find a sequence $\left\{P'_k = \prod_{i=1}^{N_k} A'_{i,k}, k \geqslant 1\right\}$ such that

$$P = \lim_{k\to\infty} P'_k, \quad \det P'_k > \tfrac{1}{2}$$

and for sufficiently large k, say $k > K$, $A'_{i,k}$ are Poisson matrices. If $\det P > \frac{1}{2}$ we simply set $P'_k = P_k$, $k \geqslant 1$. But then by the argument above $\max B'_k(n,m) \geqslant \det P'_k$ for $k > K$ and hence $\max_{(n,m)} B(n,m) \geqslant \det P$.

COROLLARY 5·1. (*Bang–Bang representation.*) *Let P be a 3×3 stochastic matrix; then P is embeddable if and only if*

$$P = \prod_{m=1}^{l} A_m.$$

Proof. An embeddable matrix P can be expressed as $P = \prod_{r=1}^{n} P_r$, where $P_1, \ldots, P_n$ are embeddable matrices and for each P_r, $1 \leqslant r \leqslant n$, $\det P_r \geqslant \frac{1}{2}$. By Theorems 4·1 and 5·1 each P_r is a product of 6 Poisson matrices.

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