Three Dimensional Line Stochastic Matrices and Extreme Points

P. Fischer and E. R. Swart Department of Mathematics and Statistics University of Guelph Guelph, Ontario, Canada

Submitted by Richard A. Brualdi

ABSTRACT

Several properties of the extreme points of the convex set of three dimensional line stochastic matrices of order n are presented. The existence of many different classes of extremal configurations is established. These extremal matrices exhibit a large variety of patterns with some unexpected configurations. Latin squares of special types are used in some of the existence results. Furthermore, three questions raised by Brualdi and Csima are answered concerning the extreme points of three dimensional plane stochastic matrices of order n.

1. INTRODUCTION

The fact that a matrix is doubly stochastic (d.s.) if and only if it is a convex combination of permutation matrices is already a part of the mathematical folklore. In other words, the permutation matrices are the extreme points of the convex and compact set of d.s. matrices (in \mathbb{R}^{n^2}). A great deal of research activity has been stimulated by this result, and by now, many proofs and generalizations of it are available.

The following two generalizations of d.s. matrices in a three dimensional setting were introduced by Jurkat and Ryser [3]:

DEFINITION 1. A three dimensional array, a matrix $A = [a_{ijk}], 1 \le i \le n$, $1 \le j \le n, 1 \le k \le n, a_{ijk} \ge 0$, is triply line stochastic (t.l.s.) if and only if the

LINEAR ALGEBRA AND ITS APPLICATIONS 69:179-203 (1985)

© Elsevier Science Publishing Co., Inc., 1985 52 Vanderbilt Ave., New York, NY 10017

0024-3795/85/\$3.30

elements of A satisfy the following equations:

$$\sum_{k=1}^{n} a_{ijk} = 1, \qquad i = 1, \dots, n, \qquad j = 1, \dots, n,$$

$$\sum_{j=1}^{n} a_{ijk} = 1, \qquad i = 1, \dots, n, \qquad k = 1, \dots, n,$$

$$\sum_{i=1}^{n} a_{ijk} = 1, \qquad j = 1, \dots, n, \qquad k = 1, \dots, n, \qquad (1)$$

and it is triply plane stochastic (t.p.s.) if and only if the elements of A satisfy the following equations:

$$\sum_{j=1}^{n} \sum_{k=1}^{n} a_{ijk} = 1, \qquad i = 1, \dots, n,$$

$$\sum_{i=1}^{n} \sum_{k=1}^{n} a_{ijk} = 1, \qquad j = 1, \dots, n,$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ijk} = 1, \qquad k = 1, \dots, n.$$
(2)

Evidently, the relation (2) implies that the sum of the elements in any one of the possible planes (a plane is a configuration for which one of the three indices is constant) is one. The relation (1) implies that each of the plane sections of A is a d.s. matrix. In particular, it implies that the sum of the elements in any one of the possible lines (a line is the intersection of two nonparallel planes) is one. It is easy to see that both of these families of matrices form a convex set for each positive integer n. The main question is to find and/or to characterize the extreme points (or the extremal matrices) of these convex sets.

The extreme points of t.p.s. matrices have been discussed by Brualdi and Csima [1], but we are not aware of any further analysis of the extreme points of t.l.s. matrices. The main topic of this paper consists of a detailed study of the extreme points of t.l.s. matrices. In addition, we answer three questions raised by Brualdi and Csima [1] concerning t.p.s. matrices. We also construct Latin squares of special types, which will be useful in establishing the existence of some special patterns.

THREE DIMENSIONAL STOCHASTIC MATRICES

2. PRELIMINARIES

For any two (three dimensional) matrices of the same order $A = [a_{ijk}]$ and $B = [b_{ijk}]$, we shall say that $A \leq B$ if $a_{ijk} \leq b_{ijk}$ for all (i, j, k), where it is assumed that the elements of the matrices are real numbers.

In the two dimensional case the positions of the unit elements of a zero-one d.s. matrix are commonly regarded as constituting a diagonal [4]. We shall say that two such diagonals are *disjoint* if they don't share a common position. Similarly, we shall say that the positions of the unit elements of a zero-one t.l.s. matrix form a triagonal.

If we consider the planes along any axis, then every triagonal is made up of a set of nonoverlapping diagonals—one in each plane. It is convenient to have special names for some of these diagonals. The diagonal consisting of the elements

$$a_{i, j, (j+k-2) \mod (n+1)+1}$$

is the k-diagonal for the *i*th (horizontal) plane. In the case of t.p.s. matrices we will follow Brualdi and Csima [1] in referring to zero-one extremal matrices as permutation matrices. It was pointed out by Jurkat and Ryser [3] that there are non-zero-one extremal t.p.s. and non-zero-one extremal t.l.s. matrices.

If A is a three dimensional matrix with real entries, its pattern Z(A) has been defined in the following way [3]:

$$Z(A) = [z_{ijk}], \quad \text{with} \quad z_{ijk} = \begin{cases} 1 & \text{when} & a_{ijk} \neq 0, \\ 0 & \text{when} & a_{ijk} = 0. \end{cases}$$

We shall denote the collection of t.l.s. matrices of order n by L_n , and the collection of t.p.s. matrices of order n by P_n .

A basic result concerning the extreme points of t.l.s. matrices has been obtained by Jurkat and Ryser [3, Theorem 3.1]. Their result is more general, but we state it below only for t.l.s. matrices.

PROPOSITION 1. A matrix $A \in L_n$ is not extremal if and only if there exists a matrix $M \neq 0$ of order n such that the sum of the elements in each line is 0 and $Z[M] \leq Z[A]$.

We shall make extensive use of this proposition and its following corollary, proven also by Jurkat and Ryser.

PROPOSITION 2. A matrix $A \in L_n$ is extremal if and only if A is the only t.l.s. matrix with pattern Z(A).

The set of $3n^2$ equations in (1) form a linearly dependent system, and it is easy to show that the rank of their coefficient matrix is $3n^2 - 3n + 1$. We can write (1) into (two dimensional) matrix form

$$Cx = b = a_{111}P_1 + \dots + a_{nnn}P_{n^3}, \qquad (3)$$

where C is the coefficient matrix of (1), of size $3n^2 \times n^3$; $x = [a_{111}, \ldots, a_{nnn}]$; $b = [1, 1, \ldots, 1]$; and P_1, \ldots, P_{n^3} are the column vectors of C. Now, if x is an extreme point of the solution set of the equation (3) (we assume, of course, that the elements of x are nonnegative), then it follows that at most $3n^2 - 3n + 1$ of the a_{ijk} are positive. (See, for instance [2, Theorem 4, p. 55].) Hence, we have the following proposition (for a different proof, see [3, p. 202]):

PROPOSITION 3. Let A be an extremal t.l.s. matrix of order n. Then the number of its positive entries, P(A), satisfies the inequality

$$P(A) \leqslant 3n^2 - 3n + 1.$$

It is easy to show by appropriate pivoting that the equations (1) are equivalent to

$$\sum_{k=1}^{n} a_{ijk} = 1, \qquad i = 1, \dots, n-1, \quad j = 1, \dots, n-1,$$
$$\sum_{j=1}^{n} a_{ijk} = 1, \qquad i = 1, \dots, n-1, \quad k = 1, \dots, n-1,$$
$$\sum_{i=1}^{n} a_{ijk} = 1, \qquad j = 1, \dots, n-1, \quad k = 1, \dots, n-1,$$
$$a_{inn} - \sum_{j=1}^{n-1} \sum_{k=1}^{n-1} a_{ijk} = 2 - n, \qquad i = 1, \dots, n-1,$$
$$a_{njn} - \sum_{i=1}^{n-1} \sum_{k=1}^{n-1} a_{ijk} = 2 - n, \qquad j = 1, \dots, n-1,$$
$$a_{nnk} - \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} a_{ijk} = 2 - n, \qquad k = 1, \dots, n-1,$$
$$a_{nnk} - \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} a_{ijk} = 2 - n, \qquad k = 1, \dots, n-1,$$

182

a

This set of equations gives a parametric solution to the original set of equations with all the a_{ijk} 's with one or more subscripts equal to n lying on the diagonal of its coefficient matrix.

If we set all the other a_{ijk} equal to zero, we get the immediate solution

$$a_{ijn} = 1, \qquad i = 1, \dots, n-1, \qquad j = 1, \dots, n-1,$$

$$a_{ink} = 1, \qquad i = 1, \dots, n-1, \qquad k = 1, \dots, n-1,$$

$$a_{njk} = 1, \qquad j = 1, \dots, n-1, \qquad k = 1, \dots, n-1,$$

$$a_{inn} = 2 - n, \qquad i = 1, \dots, n-1,$$

$$a_{njn} = 2 - n, \qquad j = 1, \dots, n-1,$$

$$a_{nnk} = 2 - n, \qquad k = 1, \dots, n-1,$$

$$a_{nnn} = n^2 - 3n + 3. \qquad (4)$$

And this proves that for all $n \ge 3$ there exists a basic solution with precisely

$$3n^2 - 3n + 1$$

nonzero elements.

It should be emphasized, however, that this is only true if we relax the nonnegativity restriction and it is not true for basic feasible solutions.

In their paper Jurkat and Ryser [3] state that:

We call the extremal matrix A and its type Z(A) maximal provided that equality holds in the appropriate corollary 3.4.

LEMMA 3.5. There exist maximal extremal arrays of size $n_1 \times n_2 \times n_3$.

The relevant inequalities are

$$P(A) \leq n_1 n_2 + n_1 n_3 + n_2 n_3 - (n_1 + n_2 + n_3) + 1$$

for line stochastic matrices, and

$$P(A) \leq (n_1 + n_2 + n_3) - 2$$

for plane stochastic matrices.

In the case $n = n_1 = n_2 = n_3$ these inequalities become

$$P(A) \leq 3n^2 - 3n + 1$$

for line stochastic matrices; and

$$P(A) \leq 3n-2$$

for plane stochastic matrices.

It is clear that Lemma 3.5 of [3] is indeed true for plane stochastic matrices with $n = n_1 = n_2 = n_3$, but it does not always hold for line stochastic matrices, since in the case n = 2 the only extrema are the two triagonals, and we thus have

$$P(A) = 4 < 3n^2 - 3n + 1 = 7.$$

In the case of n = 3, a computer assisted method shows that the only extremal t.l.s. matrices are the 6 triagonals and the 54 matrices obtained from taking all possible permutations of the three dimensional matrix

[1	0	0]	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	
0	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	
0	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	$\begin{bmatrix} 0\\ \frac{1}{2}\\ \frac{1}{2} \end{bmatrix}$	$\frac{1}{2}$	0	

This shows that the Lemma 3.5 of [3] does not hold in that case either, since max $P(A) = 17 < 3n^2 - 3n + 1 = 19$, $A \in L_3$, and A is extremal.

Since *n* is only 3, an alternative proof can be carried out by studying all possible patterns one by one. Furthermore using Proposition 2, it is simple to decide about the extremality of a given pattern. The number of patterns to be considered can be reduced by noting that, by Proposition 3, if $A \in L_3$ is extremal, then $P(A) \leq 19$. Also, Proposition 1 eliminates several possible patterns.

In discussing extremal matrices it is convenient to introduce the concept of connectedness. Two patterns P_1 and P_2 of the same type are called *independent* if there is no line which intersects both. A pattern P is connected if and only if P is not the union of two nonempty independent patterns.

There is a natural way to associate a graph G with a pattern P. We associate a node of G with each of the nonzero elements of P. Two nodes are then taken to be adjacent (i.e. connected by an edge) if and only if they lie on the same line.

It is clear that a pattern P is connected if and only if its associated graph G is connected, and the connected components of a pattern P correspond exactly to the connected subgraphs of its associated graph G.

Finally in this section, we collect some facts as lemmas about d.s. matrices which will be useful in the rest of the paper.

LEMMA 1. If D is a d.s. matrix of order n, and if the number of its positive elements is l, then the number of its unit elements (ones) is greater than or equal to 2n - l.

Proof. If D has τ units, then the remaining $n - \tau$ rows must have at least two positive elements per row; therefore

$$\tau+2(n-\tau)\leqslant l,$$

i.e.,

$$2n-l\leq\tau.$$

For easy reference the following well-known result will be called

LEMMA 2. If a $n \times n$ d.s. matrix D is not an extremal d.s. matrix, then it has a $k \times k$ submatrix with $2 \leq k \leq n$ having two disjoint diagonals.

The diagonals of such submatrices will be referred to as subdiagonals.

3. SOME SPECIAL LATIN SQUARES

In this section we shall show the existence of Latin squares of special types. These Latin squares will be useful for exhibiting interesting extremal t.l.s. matrices.

PROPOSITION 4. There exist Latin squares of the form

for n = 2 and for all $n \ge 4$.

Our proof of this proposition is constructive in nature, and is rather lengthy. Moreover, the referee has drawn our attention to an alternative and somewhat shorter proof involving conjugate pairs of partial Latin squares. We therefore present our proof in outline only.

Proof. The statement of this proposition is clearly true when n = 2, since $\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$ is a Latin square of the required type. We note also that the statement is true for $n \ge 4$ provided that we can construct a Latin square of order n such that the numbers following the unit elements of the main diagonal are all distinct.

We shall distinguish two cases, depending whether n is an even or an odd integer.

(i) The case $n = 2m \ge 4$. Consider the array $A = (a_{ij})$ of the form

$$A = \begin{bmatrix} 1 & 2 & 3 & \cdots & n \\ n & 1 & 2 & \cdots & n-1 \\ n-1 & n & 1 & \cdots & n-2 \\ \vdots & & & \vdots \\ 2 & 3 & 4 & \cdots & 1 \end{bmatrix} = (a_{ij})$$
$$= ([j-i] \mod n+1), \quad \text{where} \quad n = 2m.$$

Then it is possible by means of a joint column-row permutation of the form 1, n, 2, n-1, ..., n/2, n/2+1 to obtain an array of the desired type.

(ii) The case $n = 2m + 1 \ge 5$. In this case the above procedure does not work. It is, however, possible to start with a Latin square of the appropriate form of order 2m—constructed in the above manner—and expand it into an array of the required type of order 2m + 1.

We may note that in a Latin square B which has been constructed as above, the diagonal $b_{12}, b_{23}, \ldots, b_{n-1,n}, b_{n1}$ is such that the first n-1 elements form a permutation of the numbers $2, 3, \ldots, n$ with the element b_{n1} equal to n/2+1.

Now it can be shown that there exists another diagonal in B which shares only the position b_{n1} with this diagonal but likewise contains a permutation of the elements 2, 3, ..., n. If we replace all the elements other than b_{n1} on this second diagonal by n + 1 and add an extra row and column to the array, we can then insert the necessary additional elements to give a Latin square of order 2m + 1 of the required type.

4. SOME BASIC RESULTS

PROPOSITION 5. The maximal element in any extremal t.l.s. matrix is at least $\frac{1}{2}$.

Proof. Let $A \in L_n$ be such that each element of A is less than $\frac{1}{2}$. Then every line must have at least three positive elements. Hence $P(A) \ge 3n^2$, from which we can conclude, using Proposition 3, that A is not extremal.

PROPOSITION 6. L_n is a convex polyhedron, and its dimension is at most $(n-1)^3$. Moreover, any $A \in L_n$ can be written as the convex combination of at most $(n-1)^3 + 1$ extreme points from L_n .

Proof. The fact that L_n is a convex polyhedron is obvious, and was used before.

 $L_n \subset \mathbb{R}^{n^3}$ is in the intersection of $3n^2 - 3n + 1$ linearly independent planes; hence its dimension is at most $n^3 - (3n^2 - 3n + 1) = (n - 1)^3$. Hence L_n is a convex and compact subset of an $(n - 1)^3$ dimensional space, and by the classical Caratheodory theorem we can conclude that each $A \in L_n$ is a convex combination of at most $(n - 1)^3 + 1$ extreme points of L_n .

PROPOSITION 7. All the elements of an extremal t.l.s. matrix are rational numbers.

Proof. Let $A \in L_n$ be extremal. Then A can be obtained from (3) by Gaussian elimination, where the $3n^2 - 3n + 1$ basic variables correspond to some approximately chosen $3n^2 - 3n + 1$ linearly independent column vectors. Since the matrix C in (3) is a zero-one matrix and b = [1, ..., 1], it follows that the right hand side vector can contain only rational numbers at all stages of the Gaussian elimination.

PROPOSITION 8. If A is an extremal t.l.s. matrix, then the positions of the zero entries of A in any one plane cannot be a superset of the positions of the zero entries of a parallel plane.

Proof. If the proposition were not true, then there would exist an extremal t.l.s. matrix A such that the positions of its zero entries in the second horizontal plan (plane 2; i = 2) formed a superset of the positions of its zero entries in the top horizontal plane (plane 1; i = 1). Then the positions of the nonzero elements in plane 1 would be a superset of the positions of the

nonzero elements in plane 2, and all the elements in plane 2 would be less than 1. Hence plane 2 would not be an extremal d.s. matrix; therefore according to Lemma 2, it would have two disjoint subdiagonals. Now define the (three dimensional) matrix A_1 in the following way: 1 along one of these subdiagonals in plane 2, and -1 along the other (disjoint) subdiagonal in plane 2; in plane 1, entries -1 (1) in the same positions that were 1 (-1) in plane 2, and zero in the remaining positions. Then $Z(A_1) \leq Z(A)$ and all the line sums of A_1 are 0. Therefore, by Proposition 1, A cannot be extremal.

We introduce the following notation. Let $A \in L_n$, let k(A) be the minimum of the number of zero elements of the 3n different planes, and let

$$k_n = \min_{\substack{A \in L_n \\ A \text{ is extremal}}} k(A)$$
(5)

and

$$\tau_n = \min_{\substack{A \in L_n \\ A \text{ is connected extremal}}} k(A).$$
(6)

Now, we can prove the following proposition.

Proposition 9.

$$k_1 = 0, \qquad k_2 = 2, \qquad k_3 = 3$$

and

$$k_n \ge \left[\frac{n+1}{2}\right]$$
 for all $n \ge 4$.

Proof. For n = 1, 2, and 3 the result can be verified by inspection. Assume now that n is a fixed positive integer, $n \ge 4$. In view of the definition of k_n , there exists an extremal t.l.s. matrix A such that one of its planes has exactly k_n zero elements. Without loss of generality we can assume that it is the first horizontal plane (i = 1). Hence this plane has $n^2 - k_n$ positive elements; therefore the remaining horizontal planes have together at most

$$(3n^2 - 3n + 1) - (n^2 - k_n) = 2n^2 - 3n + k_n + 1$$

positive elements. With the aid of Lemma 1 we can conclude that the number of unit elements in the last n-1 horizontal planes is at least

$$2n(n-1) - (2n^2 - 3n + k_n + 1) = n - k_n - 1.$$

We have to distinguish some cases. If there exists among the last n-1 horizontal planes at least one plane having n unit elements, then the number of zeros in the top horizontal plane is at least n; hence in that case $k_n \ge n \ge [(n+1)/2]$.

If the number of positive elements is greater than n in each of the last n-1 horizontal planes, then there are at least n+2 positive elements in every such plane. Furthermore the number of zeros in the top horizontal plane, k_n , cannot be less than the number of unit elements in the remaining horizontal planes, i.e.

$$k_n \ge n - k_n - 1$$

Assume that $k_n = n - k_n - 1$. In that case all the zero elements in the top horizontal plane correspond to unit elements in the remaining horizontal planes. In view of Lemma 2, we can choose two disjoint subdiagonals with positive elements in the second horizontal plane, and the corresponding subdiagonals have also only positive elements in the first horizontal plane. By repeating the same argument as in the proof of Proposition 8 we can conclude that A is not an extremal matrix. Hence we must have the inequality $k_n \ge n - k_n$, which implies that $k_n \ge [(n+1)/2]$.

The previous argument can be carried further to show that if A is an extremal element of L_n with the property that no line contains exactly n-1 positive elements, then

$$k(A) \ge \left[\frac{n}{2}+1\right].$$

For τ_n the following inequality can be established.

PROPOSITION 10. $\tau_n \ge n-1$ for $n \ge 4$.

Proof. If $A \in L_n$ and if A is connected, then each of its planes has at least 2n nonzero elements. Hence if A is also extremal, then $2n(n-1) + (n^2 - \tau_n) \leq 3n^2 - 3n + 1$, i.e.

$$\tau_n \ge n-1.$$

The same proof gives the following improved result. If $A \in L_n$, and A is connected extremal, then $k(A) \ge 3n^2 - 2n - P(A)$.

In their paper [3] Jurkat and Ryser also raise the problem of characterizing those members of L_n which can be written as a convex combination of t.l.s. zero-one matrices of order n. Obviously, if $A \in L_n$ can be written as a convex combination of such matrices, then each positive entry of A lies on a positive triagonal (where we mean by a positive triagonal that each position of the triagonal is occupied by a positive element). But this condition is not sufficient. More interestingly, the following result is true.

PROPOSITION 11. For all n positive integer, $n \ge 3$, there exist t.l.s. matrices A_n and A'_n such that $Z(A_n) = Z(A'_n)$ with the property that A_n belongs to the convex hull of zero-one t.l.s. matrices of order n and A'_n does not belong to that set.

Proof. Let n be a fixed positive integer, $n \ge 3$. Let A be a non-zero-one extremal element of L_n . (The existence of such a matrix will be demonstrated later in this paper.) Let B_1, B_2, \ldots, B_n be n pairwise disjoint triagonals. Let $0 < \lambda < 1$, let

$$C_{\lambda} = \lambda A + \frac{1-\lambda}{n} (B_1 + B_2 + \cdots + B_n),$$

and let D be that member of L_n whose entries are all equal to 1/n. Then

$$Z(C_{\lambda}) = Z(D)$$
 for $0 < \lambda < 1$,

and obviously

$$D=\frac{1}{n}(B_1+\cdots+B_n).$$

Assume that the proposition is false. Let $B_1, B_2, \ldots, B_{k(n)}$ be all the possible zero-one t.l.s. matrices of order n. Then there exist nonnegative real functions $\alpha_1, \alpha_2, \ldots, \alpha_{k(n)}$ defined over the interval (0, 1) such that

$$\sum_{i=1}^{k(n)} \alpha_i(\lambda) \equiv 1 \quad \text{for} \quad \lambda \in (0,1)$$

and

$$\sum_{i=1}^{k(n)} \alpha_i(\lambda) B_i = C_\lambda \quad \text{for} \quad \lambda \in (0,1).$$

Now let $\{\lambda_m\}$ be an infinite sequence such that $\{\lambda_m\} \subset (0,1)$ and $\lambda_m \to 1$ as $m \to \infty$. By repeated application of the Bolzano-Weierstrass theorem we can conclude that there exists an infinite subsequence $\{\Gamma_j\}$ of $\{\lambda_m\}$ such that $\lim_{j\to\infty} \alpha_i(\Gamma_j)$ exists for $1 \leq i \leq k(n)$. Note that $\sum_{i=1}^{k(n)} (\lim_{j\to\infty} \alpha_i(\Gamma_j) = 1$. Clearly, we have that $A = \sum_{i=1}^{k(n)} (\lim_{j\to\infty} \alpha_i(\Gamma_j) B_i$, which is a contradiction, since A is an extremal element of L_n .

This last proposition shows that the pattern in itself is not sufficient to decide whether or not a t.l.s. matrix belongs to the convex hull of zero-one t.l.s. matrices; it depends also on the distribution of the elements. The following proposition, which can be proven easily, is a first step in that direction.

PROPOSITION 12. If $A \in L_n$ is such that each positive element of A lies on a positive triagonal and the value of each positive element is $\frac{1}{2}$, then A belongs to the convex hull of t.l.s. zero-one matrices of order n.

5. ON PLANE STOCHASTIC MATRICES

In their paper on t.p.s. matrices Brualdi and Csima [1] have raised the following questions. Let A be a connected extremal member of P_n . Does A have any of the following properties?

(1) All the positive entries of A are (integer) multiples of the smallest positive entry.

(2) The smallest positive entry is the reciprocal of an integer.

(3) If the smallest positive entry is α , then the largest entry is $1 - \alpha$, and in particular, if the maximal entry is $\frac{1}{2}$, then the smallest positive entry is likewise $\frac{1}{2}$.

With the aid of some special t.p.s. matrices together with certain appropriate constructions carried out on them, we shall answer these questions in the negative. In the following examples we shall use the notation of [1], and in Example 1 we explain this notation in detail.

EXAMPLE 1. Consider the following t.p.s. matrix:

	Eler	nents	Pla	nes
A ₁	$\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$	$\frac{1}{2}$ $\frac{1}{2}$	$\begin{bmatrix} 1\\2 \end{bmatrix}$	$\begin{bmatrix} 2\\1 \end{bmatrix}$

i.e., A_1 is a $2 \times 2 \times 2$ matrix where the top horizontal plane (plane 1) is the matrix

$$\begin{bmatrix} \frac{1}{2} & 0\\ 0 & \frac{1}{2} \end{bmatrix}$$

and the bottom horizontal plane (plane 2) is the matrix

0	$\frac{1}{2}$	
$\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}$	0	ŀ

EXAMPLE 2. Consider now the following three t.p.s. matrices:

	Elements	Planes
A_2	$\begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{2}{3} & 0 & \frac{1}{3} \\ 0 & \frac{2}{3} & \frac{1}{3} \end{bmatrix}$	$\begin{bmatrix} 1 & 1 & 2 \\ 3 & 0 & 1 \\ 0 & 2 & 3 \end{bmatrix}$
A ₃	$\begin{bmatrix} \frac{1}{6} & 0 & \frac{1}{2} & \frac{1}{3} \\ \frac{2}{3} & 0 & 0 & \frac{1}{3} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{6} & \frac{1}{2} & 0 & \frac{1}{3} \end{bmatrix}$	$\begin{bmatrix} 2 & 0 & 1 & 3 \\ 4 & 0 & 0 & 2 \\ 0 & 1 & 2 & 0 \\ 3 & 3 & 0 & 4 \end{bmatrix}$
A ₄	$\begin{bmatrix} 0 & \frac{1}{5} & \frac{2}{5} & \frac{2}{5} \\ \frac{1}{5}, \frac{1}{5} & 0 & \frac{3}{5} & 0 \\ 0 & \frac{4}{5} & 0 & \frac{1}{5} \\ \frac{3}{5} & 0 & 0 & \frac{2}{5} \end{bmatrix}$	$\begin{bmatrix} 0 & 2 & 1 & 4 \\ 1,3 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \\ 2 & 0 & 0 & 1 \end{bmatrix}$

The matrix A_3 , which is a connected extremal t.p.s. matrix, exhibits an example with minimal positive element $\alpha = \frac{1}{6}$ and with maximal element $\frac{2}{3} < 1 - \frac{1}{6}$.

Next we shall present an example of a matrix with maximal element $\frac{1}{2}$ and with minimal positive element $<\frac{1}{2}$. If all but one of the nonzero elements of A_1 are replaced by $\frac{1}{2}P$, where P is a fixed (three dimensional) permutation matrix of order 3, the remaining nonzero element is replaced by $\frac{1}{2}A_2$, and the zero elements are replaced by the $3\times3\times3$ zero matrix, then one obtains a connected extremal t.p.s. matrix of order 6. It is immediate to see that the minimal positive entry of this matrix is $\frac{1}{6}$, while the maximal one is $\frac{1}{2}$.

Consider now a similar construction applied to matrix A_2 . Assume that we replace all but one of the elements k of A_2 by kP, where P is a (three-dimensional) permutation matrix of order 4, and where the exceptional element of A_2 is one of the elements of size $\frac{2}{3}$, which is replaced by $\frac{2}{3}A_4$. Then we end up with a connected extremal t.p.s. matrix of order 12 with elements of size $\frac{2}{15}$, $\frac{4}{15}$, $\frac{1}{3}$, $\frac{2}{5}$, $\frac{8}{15}$, and $\frac{2}{3}$. Hence, for this extremal matrix the smallest positive entry $\alpha = \frac{2}{15}$ is not the reciprocal of an integer. Furthermore, there are nonzero elements, namely those of size $\frac{1}{3}$, which are not (integer) multiples of α , and the largest element is not of the form $1 - \alpha$.

6. EXISTENCE THEOREMS

In this section we shall describe certain extremal t.l.s. matrices. The construction described above in the case of plane stochastic matrices can be modified easily to give the following.

PROPOSITION 13. There exist connected extremal t.l.s. matrices for which the smallest positive element α is not of the form 1/k (where k is a positive integer); for which not all the elements are integer multiples of the smallest positive element α ; and for which the largest element is not of the form $1 - \alpha$.

In the case of d.s. matrices, the extremal matrices are the diagonals; hence every line contains only one positive element. In contrast we have

PROPOSITION 14. There exist extremal t.l.s. matrices with lines containing no zeros.

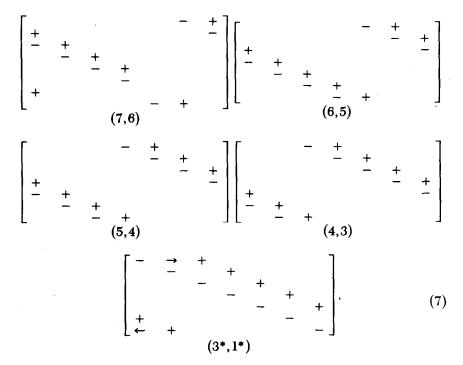
Proof. The following is an extremal matrix with the indicated properties:

The fact that it is an extremal matrix can be demonstrated with the aid of Proposition 2, i.e., one can show that it is the only t.l.s. matrix with its pattern.

The following propositions will demonstrate some unexpected features and the richness of patterns of extremal t.l.s. matrices.

PROPOSITION 15. There exist extremal t.l.s. matrices for all $n \ge 4$ with precisely $2n^2$ nonzero elements, all of which are $\frac{1}{2}$.

Proof. A construction for the case n = 7 is given below, and its generalization to all other orders ≥ 4 is explained. In what follows + and - both stand for positive numbers, and in all cases (i, j) indicates that + lies on the *i*-diagonal and - lies on the *j*-diagonal of the given plane. An asterisk * indicates a modified diagonal as explained below. The matrices in the following display represent the successive parallel vertical planes:



Clearly, in all cases (+)+(-)=1, and since in any given (vertical) plane the pattern contains two disjoint diagonals, we have that in any given plane + (and likewise -) stands for the same positive number. Note that $(1,2); (2,7); (7,6); \ldots; (3,1)$ is not an extremal pattern, since it has infinitely many different realizations, namely $\alpha = +$, with $0 < \alpha < 1$. That is why one has to modify the pattern in such a way that there exists a line containing (+)+(+)=1, which would imply $+=\frac{1}{2}=-$, the only possible realization, so that it is extremal. This has been achieved in (7) by the following transformations.

In plane 2 the diagonal 2^* is obtained from the diagonal 2 by the transformations

position $(1,2) \rightarrow$ position (1,1) (the image is on diagonal 1), position $(7,1) \rightarrow$ position (7,2) (the image is on diagonal 3);

the rest of the positions are unchanged.

In the general case, (1,2) is mapped into (1,1), $(n,1) \rightarrow (n,2)$, and the rest is unchanged.

In plane 7 the configuration on $(3^*, 1^*)$ is obtained from (3, 1) by the transformation

 $(1,1) \rightarrow (1,2)$ (image is on diagonal 2), $(7,2) \rightarrow (7,1)$ (image is on diagonal 2);

the rest of the positions are unchanged.

In the general case, in plane $n(1,1) \rightarrow (1,2), (n,2) \rightarrow (n,1)$, and the rest are unchanged.

With a slight modification of the above construction one obtains infinitely many new extremal patterns.

PROPOSITION 16. There exist extremal t.l.s. matrices for all $n \ge 5$ with precisely $2n^2 - n$ nonzero elements such that one of the planes is a zero-one d.s. matrix and the rest of the positive elements are $\frac{1}{2}$. More generally, there exist extremal t.l.s. matrices for all $n \ge 5$ with precisely $2n^2 - kn$ nonzero elements such that k of the planes are zero-one matrices and the rest of the positive elements are $\frac{1}{2}$, for all fixed k such that $1 \le k \le n - 4$.

Proof. Keeping the notation of the previous proposition, it can be seen that successive horizontal planes containing the following diagonals will form an extremal matrix with the required properties: (1,2); $(2^*, n)$; n-1; n-2;...; n-k-1; (n, n-k-2),...,(4,3), $(3^*, 1^*)$.

The next proposition will show that even more unit elements can occur in an extremal t.l.s. matrix. We shall use the following notation:

2 is a pseudodiagonal consisting of the first n-1 positions of diagonal 2 and the last position of diagonal 3 (a_{n2}) .

 $\tilde{3}$ is a set consisting of the following n-1 positions: the first n-2 positions of diagonal 3 and the last position of diagonal 2.

 $\overline{4}$ is a pseudodiagonal consisting of the first n-2 positions and the last position of diagonal 4 together with the (n-1)th position of diagonal 3.

PROPOSITION 17. There exist extremal t.l.s. matrices for all $n \ge 4$ with precisely $n^2 + 3n - 1$ nonzero elements such that n - 3 of the planes are zero-one matrices and the remaining 3 planes consisting of a single unit element and of 6n - 2 halves.

Proof. The following construction yields extremal matrices with the indicated properties. Here we enumerate the successive horizontal planes:

1; $n; n-1; \ldots; 5; (4,\tilde{3}); (3,2); (\tilde{2},\tilde{4})$. It is understood that in the (n-2)nd horizontal plane the position $a_{n-2,n-1,2}$ is 1. With another application of Proposition 2, we can see that the matrices are extremal.

We illustrate the above construction with an example when n = 6.

Example 3.

To show that even more unit elements can occur in an extremal t.l.s. matrix we need to introduce the following notation:

2° is a set consisting of the positions of diagonal 2 such that $2 \le i \le n-1$ and of the *n*th position of diagonal 3.

 $2^{\circ\circ}$ is a set consisting of the first n-2 positions of diagonal 2 and the *n*th position of diagonal 1.

1° is a set consisting of the positions of diagonal 1 such that $2 \le i \le n-1$ and of the first position of diagonal 2.

 3° is a set consisting of the first n-2 position of diagonal 3 and of the last two positions of diagonal 2.

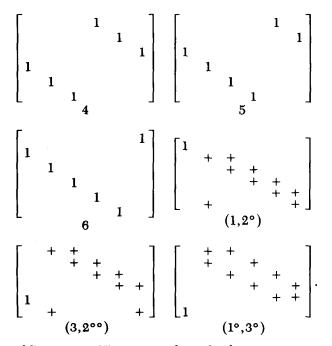
PROPOSITION 18. There exist extremal t.l.s. matrices for all $n \ge 4$ with precisely $n^2 + 3n - 3$ nonzero elements such that n - 3 of the planes are zero-one matrices and each of the remaining three planes contains 2n - 2 halves and one unit.

Proof. It can be seen, using Proposition 2, that the following matrix $(n \ge 4, n \text{ fixed})$ has the required properties (once again, we are enumerating the successive horizontal planes, indicating only the positions of the nonzero elements):

$$4;5;\ldots;n;(1,2^\circ);(3,2^{\circ\circ});(1^\circ,3^\circ).$$

We illustrate this proposition with an example when n = 6.

EXAMPLE 4.



In view of Proposition 17 it is natural to ask what is

$$\min_{\substack{A \in L_n \\ A \text{ is extremal} \\ A \text{ is not a triagonal}}} P(A) = M_n.$$

It is easy to see that $n^2 + 7 \leq M_n \leq n^2 + 3n - 3$. Furthermore, in a rather lengthy way one can show that

PROPOSITION 19. $M_4 = 4^2 + 3 \times 4 - 3 = 25.$

Our next proposition is based on the existence of certain types of Latin squares proved earlier.

PROPOSITION 20. There exist extremal t.l.s. with minimal positive element equal to 1/(n-1) for all $n \ge 2$.

Proof. Examples given already in this paper show that the result is true for n = 2, 3, and 4. Hence we can assume that n is a fixed positive integer, $n \ge 5$. The first two vertical planes will be chosen in the following way (we illustrate it in the case n = 5):

$$\begin{bmatrix} \alpha & 1-\alpha & & & \\ & \alpha & 1-\alpha & & \\ & & \alpha & 1-\alpha & \\ & & & \alpha & 1-\alpha \\ 1-\alpha & & & & \alpha \end{bmatrix}$$
$$\begin{bmatrix} 0 & \alpha & \alpha & \alpha & \alpha \\ \alpha & 1-\alpha & & \\ \alpha & & 1-\alpha & & \\ \alpha & & & 1-\alpha & \\ \alpha & & & & 1-\alpha \end{bmatrix}$$

These two planes yield the value $\alpha = 1/(n-1)$. The remaining n-2 planes will be constructed as follows. First we fill out the lower $(n-1)\times(n-1)$ submatrix in each plane in such a way that the positive entries of each of these submatrices will form a diagonal with the additional property that their perpendicular projection into the submatrix of the first horizontal plane result in n-2 disjoint diagonals, none of which intersects diagonal 1, and each of these diagonals has one and only one element from that portion of diagonal 2 which is above the main diagonal. Proposition 4 proves the existence of such diagonals. We choose the element which is on diagonal 2 to be α and the rest of the positive elements to be 1. Finally, we choose the first element of the row and the first element of the column containing α to be $1 - \alpha$ in each of these horizontal planes, and we choose a_{i11} to be α for $3 \le i \le n$. We illustrate again the remaining planes when n = 5:

$$\begin{bmatrix} \alpha & 0 & 1-\alpha & 0 & 0\\ 1-\alpha & \alpha & & & \\ 0 & & & 1\\ 0 & 1 & & & 1 \end{bmatrix} \begin{bmatrix} \alpha & & 1-\alpha & & \\ 1-\alpha & & \alpha & & \\ & 1 & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & & \\ 1-\alpha & & & & \alpha \end{bmatrix}$$

It is now evident that there is only one t.l.s. matrix with the above pattern; hence by Proposition 2, it follows that the matrix is extremal. Note that $P(A) = n^2 + 5n - 7$.

The last few results were concerned with extremal matrices $A \in L_n$ such that

$$n^2 \leqslant P(A) \leqslant 2n^2.$$

There are a large variety of extremal patterns having more than $2n^2$ positive elements.

PROPOSITION 21. For n = 4 and n = 5 and for all N such that

$$2n^2 + 1 \le N \le 3n^2 - 3n + 1$$

there exists an extremal connected t.l.s. matrix A such that P(A) = N whose positive elements are all $\frac{1}{3}$ and $\frac{2}{3}$.

Proof. It can be demonstrated by displaying the necessary examples. We shall enumerate only three cases. As previously, a possible way to show that in all of these examples the given matrices are extremal is to prove that they are the only matrices with the given pattern. To simplify the display we shall

write + instead of $\frac{2}{3}$ and - instead of $\frac{1}{3}$. We have

$$B_{1} = \begin{bmatrix} + & - & 0 & 0 \\ 0 & + & - & 0 \\ - & 0 & 0 & + \\ 0 & 0 & + & - \end{bmatrix} \begin{bmatrix} - & 0 & 0 & + \\ - & 0 & + & 0 \\ 0 & - & - & - \\ - & + & 0 & 0 \end{bmatrix}$$
$$\begin{bmatrix} 0 & + & - & 0 \\ + & 0 & 0 & - \\ - & 0 & + & 0 \\ 0 & - & 0 & + \end{bmatrix} \begin{bmatrix} 0 & 0 & + & - \\ 0 & - & 0 & + \\ - & + & 0 & 0 \\ + & 0 & - & 0 \end{bmatrix}$$

[note that $P(A) = 17 = 2 \times (4)^2 + 1$],

[note that $P(A) = 60 = 3 \times (5)^2 - 3 \times 5$], and

[note that $P(A) = 61 = 3 \times (5)^2 - 3 \times 5 + 1$].

In the light of the previous proposition following conjecture seems appropriate.

CONJECTURE 1. There exist extremal t.l.s. matrices with precisely $3n^2 - 3n + 1$ positive elements for all $n \ge 4$, and in particular, there exist connected extremal t.l.s. matrices with positive elements of size $\frac{1}{3}$ and $\frac{2}{3}$ for all N in the range $2n^2 + 1 \le N \le 3n^2 - 3n + 1$ and all $n \ge 4$, where N is the number of positive entries of the matrix.

With the aid of a random computer implementation of the simplex algorithm to the equations (1), the authors were able to find several examples of extremal t.l.s. matrices of different type with precisely $3n^2 - 3n + 1$ nonzero elements in the case n = 4. One interesting example is the following.

Example 5.

[0]	$\frac{1}{6}$	<u>5</u> 6	റി	ſ	2	0	$\frac{1}{6}$	$\frac{1}{6}$
23	$\frac{1}{3}$	0	0		$\frac{2}{3}$ $\frac{1}{3}$ 0	$ \begin{array}{c} 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{array} $	6 <u>1</u> 6	0
$\frac{2}{3}$ $\frac{1}{3}$	0	$\frac{1}{6}$	$\frac{1}{2}$		0	$\frac{1}{2}$	0	
0	$\frac{1}{2}$	0	$\frac{1}{2}$ $\frac{1}{2}$		0	0	$\frac{2}{3}$	$\frac{1}{2}$ $\frac{1}{3}$
~			-	-	_			-
$\begin{bmatrix} \frac{1}{6} \end{bmatrix}$	0	0	$\frac{5}{6}$	ſ	$\frac{1}{6}$	<u>5</u> 6	0	0]
$\begin{bmatrix} \frac{1}{6} \\ 0 \end{bmatrix}$	0 0	0 $\frac{5}{6}$	$\frac{5}{6}$ $\frac{1}{6}$	[$\frac{1}{6}$ 0	5 6 1 6	0 0	$\frac{5}{6}$
1			5 6 1 6 0		$\frac{1}{6}$ 0 $\frac{1}{3}$	5 6 1 6 0		

The following conjecture also seems probable.

CONJECTURE 2. If A is an extremal t.l.s. matrix, and if α is its smallest positive entry, then α occurs more than once in A.

This conjecture is certainly true when n = 3 or when $\frac{1}{3} \le \alpha \le \frac{1}{2}$ (of course α must be a rational number), and it is immediate to see that in that interval α must be either $\frac{1}{3}$ or $\frac{1}{2}$.

REFERENCES

1 R. A. Brualdi and J. Csima, Extremal plane stochastic matrices of dimension three, Linear Algebra Appl. 11:105–133 (1975).

THREE DIMENSIONAL STOCHASTIC MATRICES

- 2 S. I. Gass, Linear Programming, 3rd ed., McGraw-Hill, New York, 1969.
- 3 W. B. Jurkat and H. J. Ryser, Extremal configurations and decomposition theorems, J. Algebra 8:194-222 (1968).
- 4 L. Mirsky, Transversal Theory, Academic, New York, 1971.

Received 31 May 1983; revised 21 June 1984