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Multidimensional Stochastic Matrices and Patterns*

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1. INTRODUCTION

This paper deals with combinatorial properties of multidimensional stochastic matrices. Our main tool is a covering technique, developed earlier [1] for the purpose of dealing with Latin squares, doubly stochastic matrices and multidimensional (0,1) matrices. In its original form, this technique applies to covering with lines only, but the aspects required here easily generalize to covering with e-flats. The results are related to a problem of Jurkat and Ryser [3], of finding all extremal matrices within a multidimensional stochastic class. The purpose of our paper is to illuminate this fundamental problem from a new angle.

We assume a familiarity with the relevant (two-dimensional) theorems of König, Hall, and Birkhoff. Good introductions to these can be found in Ryser [6], M. Hall [4] and elsewhere. For multidimensional matrices, König's theorem is not true in the sense, that the covering number (of degree e) does not necessarily equal to the term rank (of degree e) of the matrix. This spoils the possibility of trivial generalizations of important two-dimensional theorems. Looking at the multidimensional case however, one gets a deeper insight into the two-dimensional König theory.

In Section 2.1 we define patterns as sets of lattice points, and we list some basic geometric concepts, which are natural extensions of the familiar two-dimensional ones. In Section 2.2 we introduce *crosspoints*, *restricted patterns*, and *critical patterns*. These concepts form the basis of our entire discussion about stochastic matrices.

Paragraph 3 deals with matrices. After defining (multidimensional) matrices we associate patterns with them, and extend some familiar two-dimensional concepts to higher dimensions again. In Section 3.2 we introduce stochastic matrices, and prove that stochastic matrices have restricted patterns and that

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only extremal stochastic matrices can have critical patterns. A conjecture is stated, namely that every nonempty restricted pattern is a stochastic pattern. This is true for the two-dimensional case.

In the final paragraph we give illustrative examples.

2. PATTERNS

2.1 *Basic geometric concepts*

Let J_{dn} be the set of all d tuples $(i_1, i_2, ..., i_d)$ in which the components are positive integers between 1 and n inclusive. In the rest of this paper we assume that d and n are fixed values, and exclude the trivial cases when $d = 1$ or $n = 1$. An element of J_{dn} is called a *point* or a *place*. The subsets of J_{dn} are called *patterns*. If in $(i_1, i_2, ..., i_d)$ we keep $d - e$ components fixed and let e components take up all the values from 1 to n, then the pattern (set) of the n^e points so obtained is called an *e-flat*. The only d flat is J_{dn}, the $(d - 1)$-flats are the hyperplanes, the 1-flats are the lines and the 0-flat is the empty set. In the future we assume that e is some fixed integer between 1 and $d - 1$. Two e-flats are *parallel* if they have common variable components. Two parallel e-flats are of course either identical or disjoint. *A* set of n^{d-e} distinct parallel e-flats is called a *direction*. The set of all e-flats can be partitioned into exactly $\binom{d}{e}$ directions. Let S be a pattern. Then a set L of e-flats is called a *k-cover of degree e* of S whenever $|L| = k$ and $S \subseteq \bigcup_{X \in L} X$. (*Remark.* We often suppress the expression "of degree e" but its presence in the interpretation of the text is always assumed.) If L is a c-cover of S and no k-cover of S exists with $k < c$ then we say that L is a *minimum cover* (of degree e) of S and that c is the *covering number* (of degree e) of S. A direction is of course an n^{d-e}-cover of any pattern. Hence, every pattern has at least one minimum cover and a unique covering number. Since J_{dn} has n^d points, at least n^{d-e} e-flats are required to cover J_{dn}. Hence, every direction is a minimum cover of J_{dn} and the covering number of J_{dn} is n^{d-e}.

We say that the points x and y are *independent* (of degree e) if no e-flat contains them both. The points $x_1, x_2, ..., x_p$ are said to be *independent* if they are pairwise independent. We say that the *rank* (of degree e) of a pattern S is r whenever r is the largest number such that S has a subset of r independent points. It is an immediate consequence of the definitions that the rank of a pattern can not exceed its covering number. If $d = 2$ (and necessarily $e = 1$) the well-known König theorem says that the rank and covering number of a pattern are equal. This is not true in general when $d > 2$. A *permutation pattern* of degree e (if it exists) is a pattern of n^{d-e} independent points. If a permutation pattern P is a subset of a pattern S we say that P is a *support* of S and the points of P are *supporting points* of S. It is an immediate consequence of the definitions that S has a support if and only if the rank of S is n^{d-e}.

2.2 *Restricted patterns*

We will now focus our attention on n^{d-e}-covers. The reason for this will become apparent later. In the future the noun *cover* (without prefix and without the adjective minimum) will stand for an n^{d-e}-cover. We say that the point $x \in J_{dn}$ is a *crosspoint* (of degree e) with respect to S if there exists a cover C of S and two distinct e-flats in this cover such that both contain the point x. We denote by S^{x} the set of all crosspoints with respect to S, and say that S is restricted if $S \cap S^{\mathrm{x}} = \varnothing$.

LEMMA 2.1. *The union of restricted patterns is restricted.*

Proof. Let S be the union of the restricted patterns $S_1, S_2, \ldots, S_k$. Then any cover of S is a cover of each of the S_i. If $S^{\mathrm{x}} = \varnothing$ then S is of course restricted and there is nothing left to prove. If $S^{\mathrm{x}} \neq \varnothing$ let $x \in S^{\mathrm{x}}$ be an arbitrary crosspoint with respect to S. Then also $x \in S_i^{\mathrm{x}}$ $(i = 1, 2, \ldots, k)$ since every cover of S is also a cover of S_i. But then $x \notin S_i$ $(i = 1, 2, \ldots, k)$ implies $x \notin S$ and S is restricted.

We remark here that if S is a two-dimensional pattern then $S - S^{\mathrm{x}}$ is restricted. This is not necessarily true when $d > 2$. In the next paragraph we introduce multidimensional matrices and their patterns and prove that stochastic matrices have restricted patterns. This means that we can learn about combinatorial properties of multidimensional stochastic matrices by studying restricted patterns. The concepts of crosspoints and restricted patterns (the latter with the name "reduced set") were originally introduced [1] in an attempt to isolate the supporting points of a pattern. It is clear that all the supporting points of S must lie withing $S - S^{\mathrm{x}}$. If $S - S^{\mathrm{x}} = \varnothing$ then S has no support. If S is a planar pattern $(d = 2)$ then $S - S^{\mathrm{x}}$ is restricted and the set of supporting points of S is precisely $S - S^{\mathrm{x}}$. This is not true in general when $d > 2$. In this case we can define $S_0 = S$ and $S_i = S_{i-1} - S_{i-1}^{\mathrm{x}}$ for $i = 1, 2, \ldots, m$ where m is the first positive integer such that $S_m = S_m - S_m{}^{\mathrm{x}}$. It is a simple matter to show that the supporting points of S are those of S_m. It is not true in general however that S_m is the set of supporting points of S. Since S_m is restricted it seems natural to call S_m the *restriction* of S. This definition however is not very appealing because it is given with the help of an algorithm. A more compact and far more powerful approach is to define the restriction of S as the union of its restricted subsets. We remark that the two definitions are equivalent but will not indulge ourselves in this matter any further here, because it is beyond the scope of this paper. Combinatorial properties of restricted patterns form the subject of a forthcoming paper [2] and of Chapter 5 of [1].

We say that a nonempty restricted pattern S is *critical* if S has no proper restricted subsets apart from the empty set. In view of Lemma 2.1 the union of critical patterns is restricted. When $d = 2$ the critical patterns are precisely the permutation patterns and every restricted pattern is the union of critical (i.e., permutation) patterns. When $d > 2$ there are other critical patterns besides permutation patterns and we do not know if there exists a nonempty restricted pattern which is not the union of critical patterns. Theorem 3.5 links this problem to a problem regarding patterns of stochastic matrices.

The following theorem concerns the number of points in a critical pattern.

THEOREM 2.1. *If S is a critical pattern then either S has rank n^{d-e} and S is a permutation pattern, or else the rank of S is less than n^{d-e} and $|S| > n^{d-e}$.*

Proof. Since the covering number of S is n^{d-e} we have $|S| \geqslant n^{d-e}$. Let T be an arbitrary n^{d-e}-subset of S. Then if T is a permutation pattern it is restricted and $T = S$. On the other hand if T is not a permutation pattern then there exist two distinct points $x \in T, y \in T$ in a common e-flat. It follows that the covering number of T is at most $n^{d-e} - 1$. Hence, $T \neq S$ and $|S| > |T| = n^{d-e}$.

3. MATRICES

3.1 *Multidimensional cubic matrices*

We define a matrix of order n and dimension d as a function $M : J_{dn} \to F$ where F is the field of real numbers. We say that $M(x)$ is the *entry* in M at the place or point x. A point x is a *nonzero place* of M whenever $M(x) \neq 0$. The *pattern of M* is the set of nonzero places of M. Every pattern (i.e., subset of J_{dn}) is the pattern of its own characteristic function. The characteristic functions are precisely the (0,1) matrices.

If M is a matrix, the *term rank* of M is the rank of the pattern M, and the *covering number* of M is the covering number of the pattern of M. Other concepts defined earlier in connection with patterns can be freely used in connection with matrices if there is no danger of ambiguity.

3.2 *Stochastic matrices*

We say that M is *stochastic* of degree e whenever $M(x) \geqslant 0$ for all $x \in J_{dn}$ and $\sum_{x \in S} M(x) = 1$ for all e-flats S. A stochastic matrix M is a *permutation matrix* of degree e whenever M has exactly one nonzero entry in each e-flat. It follows from the definition that permutation matrices are (0,1) matrices having permutation patterns. We say that a pattern is *stochastic* if it is the pattern of a stochastic matrix. Stochastic matrices of dimension 2 (and necessarily of degree 1) are the doubly stochastic matrices. We state without proof the next theorem, which characterizes patterns of doubly stoschastic matrices. This characterization was obtained [1, p. 6.2] independently from the (*different*) characterizations of Perfect and Mirsky [5].

THEOREM 3.1. *A two-dimensional pattern S is the pattern of a doubly stochastic matrix if and only if S is nonempty and restricted.*

For completeness we also state the characterizations of Perfect and Mirsky here.

THEOREM 3.2. (Perfect and Mirsky). *The following statements are equivalent.*

(i) *S is the pattern of a doubly stochastic matrix.*

(ii) *The* (0,1) *matrix M having pattern S can not be brought by permutation of rows and columns to the form*

$$\begin{Vmatrix} A & 0 \\ B & C \end{Vmatrix}$$

where A is of order k with $0 < k < n$, and $B \neq 0$.

(iii) *The pattern S is nonempty and every point of S is a supporting point.*

In the Perfect–Mirsky theorem both (ii) and (iii) characterize patterns of doubly stochastic matrices. The multidimensional analogue of (iii) is not true and the statement of (ii) has no immediate multidimensional analogue. Neither has the alternative statement given in a footnote of [5]. As for Theorem 3.1, we do not know whether its multidimensional analogue is true or false. We can only prove the following:

THEOREM 3.3. *Stochastic patterns are nonempty restricted patterns.*

Proof. Let M be a stochastic matrix with pattern S. Let D be a direction (i.e., a set of n^{d-e} parallel e-flats) and let C be an arbitrary cover of S. Then

$$n^{d-e} = \sum_{X \in D} \sum_{x \in X} M(x) = \sum_{x \in J_{dn}} M(x) \leqslant \sum_{X \in C} \sum_{x \in X} M(x) = \sum_{X \in C} 1 = n^{d-e} \quad (1)$$

We must have equality everywhere in (1) but this is possible only if no positive place appears in two e-flats of C. But this applies to every cover C, and we conclude that no crosspoint belongs to S and the theorem is proved.

We conjecture that the converse of Theorem 3.3 is also true. As a first step towards a proof, one should perhaps try to prove Theorem 3.1 without using König's theorem.

The next theorem is about extremal stochastic matrices. A stochastic matrix M is extremal if for $0 < \alpha < 1$ and A, B stochastic matrices the equality $M = \alpha A + (1 - \alpha)B$ holds only when $A = B = M$. The extremal doubly stochastic matrices are the permutation matrices. When $d > 2$ the permutation matrices (if they exist) are extremal but there are some other extremal matrices besides.

THEOREM 3.4. *If the pattern of a stochastic matrix M is critical then M is extremal.*

Proof. Let M be a stochastic matrix with critical pattern P such that $M = \alpha A + (1 - \alpha)B$ where A and B are stochastic matrices and $0 < \alpha < 1$. Let β be the largest entry in $B - A$. All we need to show is that $\beta = 0$. Assuming that $\beta > 0$ we define $C = \beta^{-1}(A - B + \beta B)$. Then C is stochastic with a (restricted) pattern which is a proper subset of P. This is of course a contradiction and the theorem is proved.

In the proof of the next two theorems we need the following:

LEMMA 3.1.* *Let A and B be extremal stochastic matrices with patterns S and T, respectively. Then $T \subseteq S$ if, and only if, $A = B$.*

Proof. If $A = B$, then of course $T \subseteq S$ trivially. Let us now consider the case when $T \subseteq S$. We remark that if M is an arbitrary nonnegative matrix such that $M(x) \geqslant B(x)$ for all $x \in T$, and $M \neq B$ then

$$\sum_{x \in J_{dn}} M(x) > \sum_{x \in J_{dn}} B(x) = n^{d-e}$$

and M cannot be stochastic. Hence, if we let $\alpha = \min_{x \in T} A(x)/B(x)$ then $0 < \alpha \leqslant 1$, and to prove the Lemma it suffices to show that $\alpha = 1$. Let us assume on the contrary that $0 < \alpha < 1$, and let $C = (1 - \alpha)^{-1}(A - \alpha B)$. Then C is stochastic, $A = B + (1 - \alpha)C$ and $C \neq A\,(C(y) = 0 \neq A(y)$ whenever $= A(y)/B(y))$. This contradicts the extremality of A and the proof is concluded.

We remark that if our conjecture is correct then Lemma 3.1 implies the converse of Theorem 3.4. The next theorem gives another implication.

* It was brought to our attention by the referee that our Lemma 3.1 is a trivial consequence of a corollary of Theorem 3.1 of Jurkat and Ryser (*6, p. 200, line 8 from bottom*). Jurkat and Ryser stated and proved this theorem for matrices of dimension 3 only, but indicated the possibility of generalization for higher dimensions (*6, p. 210, line 6*).

THEOREM 3.5. *If the statement that "Every nonempty restricted pattern is a stochastic pattern" is true then the following statement is also true. "Every nonempty restricted pattern is the union of critical patterns."*

Proof. Let us assume that every nonempty restricted pattern is a stochastic pattern. Let S be the pattern of the stochastic matrix A. Then A is the convex combination of some extremal matrices $A_1, A_2, ..., A_k$ with patterns $S_1, S_2, ..., S_k$. But then $A = \sum_{i=1}^{k} \alpha_i A_i$, $\alpha_i > 0$ $i = 1, 2, ..., k$ implies $S = \bigcup_{i=1}^{k} S_i$. It follows from our remark after the proof of Lemma 3.1 that $S_1, S_2, ..., S_k$ are critical, and the proof is concluded.

We remark here that if our conjecture is correct then the minimal types of Jurkat and Ryser [3] are precisely the characteristic functions of our critical patterns. We would like to emphasize however that while the definition of a minimal type depends on the definition of a stochastic class and on the existence of at least one stochastic matrix with the type in question, critical patterns are defined by simple covering criteria which do not depend for instance on the addition of real numbers.

Our final theorem is analogous to Theorem 2.1.

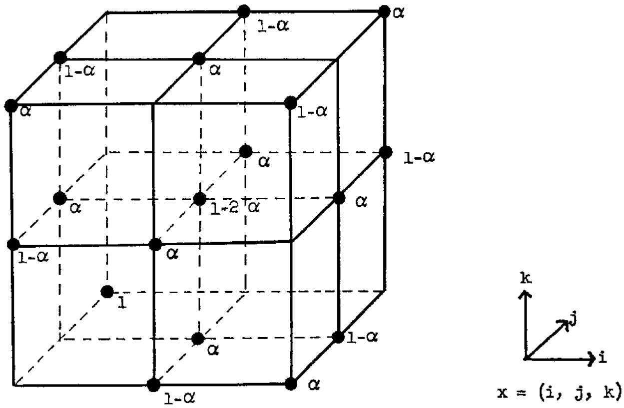
THEOREM 3.6. *If M is an extremal stochastic matrix then either M is a permutation matrix or else the term rank of M is less than n^{d-e} and M has more than n^{d-e} positive entries.*

Proof. Let S be the pattern of M. Then S has a critical pattern T as a subset. If T is a permutation pattern then its characteristic function is a permutation matrix and it follows from Lemma 3.1 that $T = S$ and M is a permutation matrix. If T is not a permutation pattern then from Theorem 2.1 $n^{d-e} < |T| \leqslant |S|$ and the proof is concluded.

4. EXAMPLES

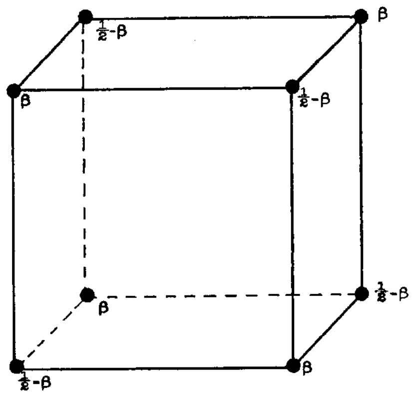
The matrix A_α of Fig. 1 is a three-dimensional line-stochastic (i.e., stochastic of degree 1) matrix for $0 \leqslant \alpha \leqslant 1/2$. The matrices A_0 and $A_{1/2}$ are both extremal, but only A_0 is a permutation matrix. Observe, that $A_{1/2}$ has term rank 8 and covering number 9.

The matrix B_β in Fig. 2 is a three-dimensional plane-stochastic (i.e. stochastic of degree 2) matrix for $0 \leqslant \beta \leqslant 1/2$. The matrices B_0 and $B_{1/2}$ are both extremal, but none of them is a permutation matrix. They both have term rank 1 and covering number 2. The matrix $B_{1/4}$ is the convex combination of B_0 and $B_{1/2}$, but $B_{1/4}$ is also the convex combination of four permutation matrices.



x	$A_\alpha(x)$	x	$A_\alpha(x)$
(1, 1, 2)	$1-\alpha$	(1, 1, 3)	α
(1, 2, 2)	α	(1, 2, 3)	$1-\alpha$
(1, 3, 3)	1	(2, 1, 1)	$1-\alpha$
(2, 1, 2)	α	(2, 2, 1)	α
(2, 2, 2)	$1-2\alpha$	(2, 2, 3)	α
(2, 3, 2)	α	(2, 3, 3)	$1-\alpha$
(3, 1, 1)	α	(3, 1, 3)	$1-\alpha$
(3, 2, 1)	$1-\alpha$	(3, 2, 2)	α
(3, 3, 2)	$1-\alpha$	(3, 3, 3)	α

Figure 1.



x	$B_\beta(x)$
(1, 1, 1)	$\frac{1}{2}-\beta$
(1, 1, 2)	β
(1, 2, 1)	β
(1, 2, 2)	$\frac{1}{2}-\beta$
(2, 1, 1)	β
(2, 1, 2)	$\frac{1}{2}-\beta$
(2, 2, 1)	$\frac{1}{2}-\beta$
(2, 2, 2)	β

Figure 2.

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