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G. Dahl* and T. A. Haufmann

Zero-one completely positive matrices and the $\mathcal{A}(R, S)$ classes

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Abstract: A matrix of the form $A = BB^T$ where B is nonnegative is called completely positive (CP). Berman and Xu (2005) investigated a subclass of CP-matrices, called $\{0, 1\}$ -completely positive matrices. We introduce a related concept and show connections between the two notions. An important relation to the so-called cut cone is established. Some results are shown for $\{0, 1\}$ -completely positive matrices with given graphs, and for $\{0, 1\}$ -completely positive matrices constructed from the classes of $(0, 1)$ -matrices with fixed row and column sums.

Keywords: Completely positive matrix, $(0, 1)$ -matrix, convex cone

1 Introduction

$M_{n,k}$ (resp. M_n) denotes the set of real $n \times k$ (resp. $n \times n$) matrices, and \mathbb{R}_+ denotes the set of nonnegative real numbers. \mathcal{B}_n denotes the set of n -dimensional $(0, 1)$ -vectors, and $\mathcal{B}_{n,k}$ denotes the set of $n \times k$ $(0, 1)$ -matrices. For a set S of vectors, cone S is the conical hull of S (the set of linear combinations with nonnegative coefficients).

A matrix $A \in M_n$ is called *completely positive*, or simply a *CP-matrix*, if it has a factorization $A = BB^T$ where B is a nonnegative matrix in $M_{n,k}$ for some positive integer k . The *CP-cone* \mathcal{C}_n^* is the set of $n \times n$ CP-matrices. \mathcal{C}_n^* is a full-dimensional, closed convex cone in the space of symmetric $n \times n$ matrices; see [1] for a proof of these and other facts concerning the CP-cone. The extreme rays of \mathcal{C}_n^* are generated by the rank-one matrices xx^T where $x \geq 0$ (where 0 denotes the zero vector). The dual of the CP-cone is the copositive cone, and optimization problems over both of these cones have been extensively investigated, see for example [5, 6, 9].

This paper deals with different subsets of \mathcal{C}_n^* . In particular, we consider matrices A that have a factorization $A = BB^T$ where B is a $(0, 1)$ -matrix. This is a special case of binary matrix factorization, see [13]. In [2] complete positivity was extended as follows: For a nonempty set $S \subseteq \mathbb{R}_+$, a matrix $A \in M_n$ is called *S-completely positive* if $A = BB^T$ where $B = [b_{ij}] \in M_{n,k}$ for some k and $b_{ij} \in S$ ($i \leq n, j \leq k$). The classical notion of complete positivity corresponds to $S = \mathbb{R}_+$. Clearly, if a matrix is S -completely positive, it is also a CP-matrix. As in [2] (see also [3]) we shall focus on the case $S = \{0, 1\}$, which gives the notion of a $\{0, 1\}$ -completely positive matrix, or a $\{0, 1\}$ -CP matrix, for short. A goal of this paper is to supplement the analysis in [2, 3] by exploiting a connection to the so-called cut cone.

We now define a new class of CP-matrices. We say that a matrix A is a $CP^{0,1}$ -matrix if

$$A = \sum_{i=1}^k \lambda_i b_i b_i^T, \quad (1)$$

where k is an arbitrary positive integer, $\lambda_i \geq 0$ and $b_i \in \mathcal{B}_n$ for $i \leq k$. The set of all $CP^{0,1}$ -matrices is denoted by $\mathcal{CP}_n^{0,1}$, and this set is called the $CP^{0,1}$ -cone. This is a finitely generated convex cone, and it is generated by

*Corresponding Author: G. Dahl: Department of Mathematics, University of Oslo, Oslo, Norway, E-mail: geird@math.uio.no
T. A. Haufmann: Department of Mathematics, University of Oslo, Oslo, Norway, E-mail: torkelah@math.uio.no

the set Cor_n consisting of the $2^n - 1$ rank one matrices of the form bb^T for nonzero $b \in \mathcal{B}_n$, so

$$\mathcal{CP}_n^{0,1} = \text{cone Cor}_n.$$

For any matrix B , $BB^T = \sum_{i=1}^k b_i b_i^T$ where b_1, b_2, \dots, b_k are the columns of B , so it follows that any $\{0, 1\}$ -completely positive matrix is also a $\mathcal{CP}_n^{0,1}$ -matrix. This gives the inclusions

$$\text{Cor}_n \subseteq \{A \in M_n : A \text{ is a } \{0, 1\}\text{-CP matrix}\} \subseteq \mathcal{CP}_n^{0,1} \subseteq \mathcal{C}_n^*.$$

From convexity (the main theorem for polyhedra), as $\mathcal{CP}_n^{0,1}$ is a finitely generated convex cone, it is also a polyhedron. This means that there is a (finite) linear system of inequalities whose solution set equals $\mathcal{CP}_n^{0,1}$.

Throughout, all graphs are assumed to be undirected. If i and j are vertices in a graph we will denote the edge connecting them by ij or ji . For a symmetric $n \times n$ matrix A , its *graph* $G(A)$ has vertex set $\{1, 2, \dots, n\}$ and an edge ij if $a_{ij} \neq 0$. The graph of A thus describes the zero pattern of A .

The rest of this paper is organized as follows: In Section 2 we discuss $\mathcal{CP}_n^{0,1}$ and some connections to previous work, and Section 3 deals with the relation between $\{0, 1\}$ -complete positivity and the graph of a matrix. In Section 4 we discuss the set of $\{0, 1\}$ -completely positive matrices obtained as an image of the $(0, 1)$ -matrices with given row and column sums.

We let \mathbb{R}^n (\mathbb{R}_+^n) denote the set of n -dimensional real (nonnegative) n -tuples, and identify this with column vectors. \mathbb{Z}^n and \mathbb{Z}_+ are defined analogously. For any set S , \mathbb{R}^S denotes the set of functions from S into \mathbb{R} . The *support* of a vector $x \in \mathbb{R}^n$ is $\text{supp } x = \{i : x_i \neq 0\}$. By a *line* of a matrix we mean either a row or a column. For matrices $A, B \in M_n$, we use the Frobenius inner product $\langle A, B \rangle = \sum_{ij} a_{ij} b_{ij}$. If A and B are matrices of the same size, $A \geq B$ (or $B \leq A$) means that this inequality holds for all entries. O is the zero matrix. A matrix A is nonnegative if $A \geq O$. \mathcal{S}_n is the space of symmetric matrices in M_n , and \mathcal{S}_n^+ denotes the nonnegative symmetric matrices in M_n . e is the vector of all ones, where the dimension is clear from the context. Similarly e_i denotes the i -th column of the identity matrix. If S is a finite set, its cardinality is denoted by $\#S$ or $|S|$. We write $[1 : n]$ for the set $\{1, 2, \dots, n\}$.

2 The correlation cone

We now observe that $\mathcal{CP}_n^{0,1}$, under a different name, has been investigated in the area of polyhedral combinatorics and discrete geometry. In particular, the book [8] contains many relevant results. In order to make this connection clear we review some central concepts and results from [8], on which the next three paragraphs are based.

For a positive integer n , define $E_n = \{ij : 1 \leq i < j \leq n\}$ and $\bar{E}_n = \{ij : 1 \leq i \leq j \leq n\}$. We think of E_n as the edges of a complete (undirected) graph with n vertices, and without loops, while \bar{E}_n also has elements corresponding to the vertices of the graph, identifying ii with i . A function $w : \bar{E}_n \rightarrow \mathbb{R}$ defines a symmetric matrix $A = [a_{ij}] \in \mathcal{S}_n$ such that $a_{ij} = a_{ji} = w_{ij}$ when $i \leq j$, and vice versa. For any $I \subseteq [1 : n]$, define the *correlation vector* $\chi^I \in \mathbb{R}^{\bar{E}_n}$ by $\chi_{ij}^I = 1$ if $i \leq j$ and $i, j \in I$, and 0 otherwise.

The cone $\text{COR}_n = \text{cone}\{\chi^I : I \subseteq [1 : n]\} \subseteq \mathbb{R}^{V_n \cup E_n}$ is known as the *correlation cone*. There is a 1-1 correspondence between the set Cor_n (defined in the previous section) and the set of correlation vectors of length n : If $A = bb^T \in \text{Cor}_n$ where b is a $(0, 1)$ -vector, then $\chi^I \in \text{COR}_n$ where $I = \text{supp } b$. Similarly one constructs a matrix $A \in \text{Cor}_n$ for any correlation vector χ^I . Therefore, there is a 1-1 correspondence between the $\mathcal{CP}_n^{0,1}$ -cone and the correlation cone COR_n .

Next, for $S \subseteq [1 : n]$ define the *cut vector* $\delta \in \mathbb{R}^{E_n}$ by

$$\delta_{ij}^S = \begin{cases} 1 & \text{if } |\{i, j\} \cap S| = 1, \\ 0 & \text{otherwise.} \end{cases}$$

The *cut cone* is defined as $\text{CUT}_n = \text{cone}\{\delta^S : S \subseteq [1 : n]\} \subseteq \mathbb{R}^{E_n}$. One reason for the interest in the cut cone is that the maximum cut problem, a well-known combinatorial optimization problem, may be formulated as

a linear optimization problem over the *cut polytope*, defined as the convex hull of all cut vectors, see again [8]. The cut polytope and the cut cone are closely related. Therefore, valid linear inequalities for the cut polytope (i.e., inequalities satisfied by all points in the cut polytope) may be used for obtaining bounds for, or sometimes solving, the maximum cut problem.

The cut and correlation cones are closely related, as described next.

Theorem DL1. [8] *Let the linear map $T : \mathbb{R}^{E_{n+1}} \rightarrow \mathbb{R}^{\bar{E}_n}$ be defined by $y = T(\delta)$ where $\delta \in \mathbb{R}^{E_{n+1}}$ and*

$$y_{ii} = \delta_{i,n+1} \quad \text{if } 1 \leq i \leq n,$$

$$y_{ij} = \frac{1}{2}(\delta_{i,n+1} + \delta_{j,n+1} - \delta_{ij}) \quad \text{if } 1 \leq i < j \leq n.$$

Then T is an isomorphism and the image of CUT_{n+1} under this map is COR_n .

The map T is called the *covariance mapping*. The separation problem for the cut cone is NP-hard, see [10]. Using the covariance mapping, it is clear that the separation problem for the correlation cone is also NP-hard, and by the isomorphism between the correlation cone and the $CP^{0,1}$ -cone, it follows that the separation problem for the $CP^{0,1}$ -cone is NP-hard.

The cone CUT_n has a very complicated facial structure, and only some classes of facets are known in general. In some special cases a complete linear description is known. For instance, [8] describes inequalities defining *all* facets of CUT_n for $n \leq 7$. In light of the covariance mapping and the relation between $CP_n^{0,1}$ and the correlation cone, this leads to a complete linear inequality description of $CP_n^{0,1}$ for $n \leq 6$. We now discuss consequences of this connection, for small values of n . Translating the correlation cone inequalities into inequalities for $CP_n^{0,1}$ is straightforward, and we omit these details.

First, for $n = 2$, one checks that $A \in CP_2^{0,1}$ if and only if A is nonnegative and diagonally dominant. For $n = 3$ we obtain the following result - see further discussion below.

Corollary 2.1. *Let $A \in S_3$. Then $A \in CP_3^{0,1}$ if and only if*

$$a_{ij} \geq 0, \quad a_{ii} \geq a_{ij}, \quad a_{ij} \geq a_{ik} + a_{kj} - a_{kk},$$

for any distinct indices i, j, k in $\{1, 2, 3\}$.

By inspection of the generators of $CP_3^{0,1}$, one verifies that all inequalities in Corollary 2.1 are in fact necessary, but the sufficiency is more complicated.

Consider an inequality in Corollary 2.1, written as $\sum_{ij} b_{ij} a_{ij} \geq 0$ where $b_{ij} \in \{0, 1, -1\}$. It may be represented graphically as follows. We represent $b_{ij} = 1$ with a + sign and $b_{ij} = -1$ with a - sign, and omit zeroes. Due to symmetry we only indicate positions in the upper triangular part of a matrix.

$$\begin{aligned}
 a_{ij} \geq 0 : & \quad \begin{bmatrix} & + & \\ & & \\ & & \end{bmatrix}, \quad \begin{bmatrix} & & + \\ & & \\ & & \end{bmatrix}, \quad \begin{bmatrix} & & \\ & & \\ & & + \end{bmatrix} \\
 a_{ii} \geq a_{ij} : & \quad \begin{bmatrix} + & - & \\ & & \\ & & \end{bmatrix}, \quad \begin{bmatrix} + & & - \\ & & \\ & & \end{bmatrix}, \quad \begin{bmatrix} & & \\ & + & - \\ & & \end{bmatrix}, \dots \tag{2} \\
 a_{ij} \geq a_{ik} + a_{kj} - a_{kk} : & \quad \begin{bmatrix} + & - & - \\ & & + \\ & & \end{bmatrix}, \quad \begin{bmatrix} & - & + \\ & + & - \\ & & \end{bmatrix}, \quad \begin{bmatrix} & + & - \\ & & - \\ & & + \end{bmatrix}
 \end{aligned}$$

We see that the last type of inequality in Corollary 2.1 is a kind of weakened diagonal dominance inequality. In fact, all the inequalities in Corollary 2.1 belong to the same class of inequalities – they all appear as the images of the so-called triangle inequalities for CUT_4 . We remark that triangle inequalities for the cut cone reflect that cuts correspond to special metrics on a finite set. For higher dimensions further classes of inequalities are needed.

Corollary 2.2. *Let $A \in \mathcal{S}_4$. Then $A \in \mathcal{CP}_4^{0,1}$ if and only if the following inequalities hold for any distinct indices i, j, k, l in $\{1, 2, 3, 4\}$:*

– Triangle inequalities:

$$a_{ij} \geq 0, \quad a_{ii} \geq a_{ij}, \quad a_{ij} \geq a_{ik} + a_{kj} - a_{kk}.$$

– Taking the left sum over $r \neq i, s \neq i, r \neq s$ and the right sum over $s \neq i$:

$$\sum_{r,s} a_{rs} \geq \sum_s a_{is} - a_{ii}.$$

– If $i < j, k < l$ and the sum is over $rs \neq ij, rs \neq kl, r \neq s$:

$$a_{ij} + a_{kl} \geq \sum_{r,s} a_{rs} - a_{kk} - a_{ll}.$$

We may now relate our notion of $\mathcal{CP}^{0,1}$ -matrices and the Berman-Xu notion of $\{0, 1\}$ -CP matrices.

Proposition 2.3. *All integer matrices in $\mathcal{CP}_n^{0,1}$ are $\{0, 1\}$ -CP if and only if $n \leq 4$.*

Proof. This is obtained directly from Corollary 2 of [11]. □

So, for $n \geq 5$, there are integral $\mathcal{CP}^{0,1}$ -matrices that are not $\{0, 1\}$ -CP matrices, and such an example (see [11]) is:

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

Our discussion leads to the following characterizations of $\{0, 1\}$ -CP matrices for $n \leq 4$. As mentioned above, if $n = 2$ the $\{0, 1\}$ -CP matrices are precisely the integral nonnegative diagonally dominant ones.

Corollary 2.4.

- (a) *A matrix of order 3 is $\{0, 1\}$ -CP if and only if it satisfies the inequalities in Corollary 2.1.*
- (b) *A matrix of order 4 is $\{0, 1\}$ -CP if and only if it satisfies the inequalities in Corollary 2.2.*

Proof. Apply Proposition 2.3 to Corollaries 2.1 and 2.2. □

Corollary 2.4 (a) is Theorem 2.2 in [2]. Corollary 2.4 (b) generalizes Theorem 4.2 in [2] since that theorem only considers matrices of order 4 with at least one zero entry.

We noted above that in [8] there is a full description of CUT_n for $n \leq 7$ and therefore also COR_n for $n \leq 6$, but we have only used this result for $n \leq 4$. In light of Proposition 2.3 we cannot hope to prove a result such as Corollary 2.4 for $n = 5, 6$, but we may obtain analogues of Corollaries 2.1 and 2.2. The reason for avoiding this here is that the description of CUT_n grows rapidly in complexity as n increases, and explicitly listing the inequalities would be unwieldy.

3 $\{0, 1\}$ -CP matrices with given graphs

We now consider $\{0, 1\}$ -CP matrices with special zero patterns. A goal is to obtain stronger results (for instance, characterizations) when special structure is present. We refer to [3] for some related ideas and results.

Theorem 3.1. *Let $A \in \mathcal{S}_n$ be a matrix such that $G(A)$ is a tree. Then A is $\{0, 1\}$ -CP if and only if A is diagonally dominant.*

Proof. If A is $\{0, 1\}$ -CP, it has a rank 1 representation

$$A = \sum_{i=1}^k \lambda_i b_i b_i^T, \quad \text{where } \lambda_i \in \mathbb{Z}_+, b_i \in \mathcal{B}_n \text{ for } i \leq k. \tag{3}$$

Then, if $|\text{supp } b_i| > 2$ for some i , the graph of A cannot be a tree, as for each i , b_i gives rise to a clique in $G(A)$, and any clique of size greater than 2 contains a cycle. Then each $b_i b_i^T$ in (3) is taken from the set

$$\{e_i e_i^T : i = 1, 2, \dots, n\} \cup \{(e_i + e_j)(e_i + e_j)^T : 1 \leq i, j \leq n, i \neq j\}.$$

As all these matrices are diagonally dominant (see [7]), it follows that A is diagonally dominant.

Conversely, if A is nonnegative, integral and diagonally dominant, consider the representation

$$A = \sum_{i=1}^n r_i e_i e_i^T + \sum_{i < j} a_{ij} (e_i + e_j)(e_i + e_j)^T$$

where $r_i = a_{ii} - \sum_{j \neq i}^n a_{ij}$. Then, by the assumptions, all coefficients in this sum are nonnegative, and so A is $\{0, 1\}$ -CP. □

We remark that the if-part of this proof is well known, and also holds when the graph is not a tree (see for example [1]). Theorem 3.2 in [2] is a special case of Theorem 3.1.

It is possible to strengthen Theorem 3.1. By a *triangle* in a graph we mean a cycle of length 3.

Theorem 3.2. *Let A be an integral, symmetric and nonnegative matrix such that $G(A)$ contains no triangles. Then A is $\{0, 1\}$ -CP if and only if A is diagonally dominant.*

Proof. The proof is similar to that of Theorem 3.1: Any $b \in \mathcal{B}_n$ gives rise to a clique in $G(A)$, and if the cardinality of $\text{supp } b$ exceeds 2, such a clique contains a triangle. □

This result is in fact a characterization of all triangle-free graphs, as we now show. The result is an analogue of Theorem 2.9 in [1]. Consider the following property of a graph G :

(DD) For every nonnegative symmetric matrix A with $G(A) = G$, A is $\{0, 1\}$ -CP if and only if A is diagonally dominant.

Theorem 3.3. *A graph G satisfies property (DD) if and only if G is triangle-free.*

Proof. If G is triangle-free, then property (DD) holds by Theorem 3.2.

Next, assume G has this property and that vertices 1, 2, 3 in G induce a triangle. Say G has n vertices, and let $A \in \mathcal{S}_n$ be defined by

$$a_{ij} = \begin{cases} 1 & \text{if } i, j \leq 3, \\ 0 & \text{otherwise.} \end{cases}$$

Then $A = (e_1 + e_2 + e_3)(e_1 + e_2 + e_3)^T$ is $\{0, 1\}$ -CP, yet A is not diagonally dominant. □

Our next result contains a reduction principle for determining whether or not a matrix is $\{0, 1\}$ -CP. It is analogous to Lemma 2.2 in [1].

Theorem 3.4. *Let $A \in \mathcal{S}_n^+$ be an integral matrix and let $\{i, j\}$ be an edge of $G(A)$ that does not lie in a triangle. Then A is $\{0, 1\}$ -CP if and only if*

$$A - a_{ij}(e_i + e_j)(e_i + e_j)^T$$

is $\{0, 1\}$ -CP.

Proof. The “if” part of the proof is trivial.

If A is $\{0, 1\}$ -CP, A has a rank 1 representation

$$A = \sum_{s=1}^k \lambda_s b_s b_s^T, \quad \text{where } \lambda_s \geq 0, b_s \in \mathcal{B}_n \text{ for } s \leq k. \tag{4}$$

For any b_s in (4), if $\{i, j\} \subseteq \text{supp } b_s$, then $\text{supp } b_s = \{i, j\}$. Otherwise, there would be some $l \in \text{supp } b_s \setminus \{i, j\}$, and $G(A)$ would contain the triangle (ij, jl, li) , contradicting the assumptions on $\{i, j\}$. Hence $(b_s b_s^T)_{ij} \neq 0$ if and only if $b_s = (e_i + e_j)$. Without loss of generality we can assume there is only one such term in the rank 1 representation, and that it is b_k . Clearly, $\lambda_k = a_{ij}$.

Let

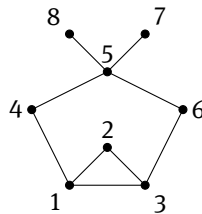
$$A' = \sum_{s=1}^{k-1} \lambda_s b_s b_s^T.$$

Then $A = A' + a_{ij}(e_i + e_j)(e_i + e_j)^T$, and A' is $\{0, 1\}$ -CP, which concludes the proof. □

As an example, consider the matrix

$$A = \begin{bmatrix} 6 & 1 & 3 & 2 & 0 & 0 & 0 & 0 \\ 1 & 2 & 2 & 0 & 0 & 0 & 0 & 0 \\ 3 & 2 & 8 & 0 & 0 & 3 & 0 & 0 \\ 2 & 0 & 0 & 3 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 7 & 1 & 1 & 2 \\ 0 & 0 & 3 & 0 & 1 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 \end{bmatrix}.$$

This matrix can not be shown to be $\{0, 1\}$ -CP by any of the techniques discussed previously: It has order greater than 4, it is not diagonally dominant and its graph is not a tree. This is $G(A)$:



The only edges of $G(A)$ that lie in a triangle are $\{1, 2\}$, $\{2, 3\}$ and $\{1, 3\}$. Repeated applications of Theorem 3.4 show that A is $\{0, 1\}$ -CP if and only if

$$A' = \begin{bmatrix} 4 & 1 & 3 \\ 1 & 2 & 2 \\ 3 & 2 & 5 \end{bmatrix}$$

is $\{0, 1\}$ -CP, which can be easily seen to be the case, for example by using Corollary 2.4 (a).

Combining Theorem 3.4 with the subgraphs for which characterizations are known, one can determine $\{0, 1\}$ -complete positivity for a range of matrices.

4 Ryser classes and $\{0, 1\}$ -CP matrices

The definition of $\{0, 1\}$ -complete positivity is given in terms of $(0, 1)$ -matrices. In this section we study matrices BB^T where B is a $(0, 1)$ -matrix with given row and column sums.

We recall the notion of majorization: If a, b are nonnegative nonincreasing vectors of dimension n , a is majorized by b , written $a \preceq b$, if

$$\sum_{i=1}^k a_i \leq \sum_{i=1}^k b_i \text{ for } k = 1, 2, \dots, n-1, \text{ and } \sum_{i=1}^n a_i = \sum_{i=1}^n b_i.$$

If a is a nonnegative nonincreasing integer vector, its *conjugate* vector a^* (of suitable length) is defined by

$$a_k^* = |\{i : a_i \geq k\}|.$$

A *transfer* on a consists in subtracting 1 in some position i and adding 1 in another position $j > i$ with $a_i > a_j + 1$ (we permit $j = n + 1$). If $a \preceq b$, we may obtain b from a by a sequence of transfers – see [4].

If R and S are nonnegative nonincreasing integral vectors of length n and p , respectively, $\mathcal{A}(R, S)$ is defined as the set of matrices in $\mathcal{B}_{n,p}$ with row sum vector R and column sum vector S .

Let f denote the mapping $X \mapsto XX^T$. So, the set of $\{0, 1\}$ -completely positive matrices is the image under f of all $(0, 1)$ -matrices. We define

$$\mathcal{F}(R, S) = f(\mathcal{A}(R, S)).$$

Our goal is to investigate the cardinality of $\mathcal{F}(R, S)$ and, in particular, when there is only one matrix in this class. The Gale-Ryser theorem (see [4]) says that $\mathcal{A}(R, S)$ is nonempty if and only if $S \preceq R^*$. If $S = R^*$, there is a unique matrix in $\mathcal{A}(R, S)$. $\mathcal{F}(R, S)$ inherits these properties.

A matrix A is $\{0, 1\}$ -CP if and only if PAP^T is $\{0, 1\}$ -CP for any permutation matrix P . Furthermore, if $A = BB^T$ where B is a $(0, 1)$ -matrix, A is unchanged by column permutations of B , so we may assume such a B has nonincreasing column sums. Therefore we have

$$A \text{ is } \{0, 1\}\text{-CP} \Leftrightarrow PAP^T \in \mathcal{F}(R, S) \text{ for some } R, S \text{ and permutation matrix } P.$$

The diagonal of A is the row sum vector of B , so the required permutation matrix P is chosen to make the diagonal of PAP^T nonincreasing.

In the remainder of the section we assume that R and S are nonnegative nonincreasing integral vectors with $S \preceq R^*$, so $\mathcal{A}(R, S)$ is nonempty. Now choose $A \in \mathcal{F}(R, S)$. Then the diagonal of A equals R , but S does not appear explicitly in A , although $e^T A e = S^T S$.

Proposition 4.1. *If $A \in \mathcal{F}(R, S)$ and $A \in \mathcal{F}(R, S')$ where S' is a nonnegative nonincreasing integral vector (so $S, S' \preceq R^*$) and $S \neq S'$, then neither of S and S' majorizes the other.*

Proof. Assume $S \preceq S'$. Then S can be obtained from S' by a sequence of transfers. Inspection of the elements of S shows that a transfer strictly reduces the inner product $S^T S$, which means that $S^T S < (S')^T (S')$. This is a contradiction, as $S^T S = e^T A e = (S')^T (S')$. □

If B, \bar{B} are matrices in $\mathcal{A}(R, S)$, \bar{B} may be obtained from B by a sequence of *interchanges* (see [4]). An interchange consists in replacing a submatrix which is equal to the 2×2 identity matrix, I_2 , by the matrix

$$L_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

or vice versa. Let i_1, i_2, j_1, j_2 be indices and let $B[i_1, i_2; j_1, j_2]$ be the submatrix of B with rows indexed by i_1, i_2 and columns by j_1, j_2 . Then if $B[i_1, i_2; j_1, j_2] = I_2$ we may apply an interchange, obtaining a new matrix $B' \in \mathcal{A}(R, S)$. Let $M = f(B') - f(B)$, and let $b' = b_{j_2} - b_{j_1}$, where b_i denotes the i -th column of B . Then M is a matrix which is zero everywhere except in the lines indexed by i_1 or i_2 . Row and column i_1 are equal to b' , while row and column i_2 are equal to $-b'$, excepting the intersections of these lines, where we have

$$M_{i_1 i_1} = M_{i_2 i_2} = M_{i_1 i_2} = M_{i_2 i_1} = 0.$$

If there is some $t \in \text{supp } b_{j_1} \triangle \text{supp } b_{j_2}$ (the symmetric difference) with $t \neq i_1, t \neq i_2$, it follows that M is nonzero, and $f(B') \neq f(B)$. If there is no such t , then the interchange can also be represented by a column permutation, i.e., there is a permutation matrix P such that $B' = BP$. This discussion shows the following result.

Proposition 4.2. $\#\mathcal{F}(R, S) = 1$ if and only if for all $B \in \mathcal{A}(R, S)$ each possible interchange corresponds to a column permutation.

In terms of the support of the columns, $\#\mathcal{F}(R, S) > 1$ if and only if there are two columns b_i and b_j in B such that

$$|\text{supp } b_i \setminus \text{supp } b_j| \geq 1, |\text{supp } b_j \setminus \text{supp } b_i| \geq 1, |\text{supp } b_i \triangle \text{supp } b_j| \geq 3. \tag{5}$$

This property is either possessed by all matrices in $\mathcal{A}(R, S)$ or none of them – one only needs to check a single matrix in the class.

We remark that the condition in Proposition 4.2 is strong. For example, let $R = (2, 1, 1, 1, 1), S = (3, 3)$ and observe that both

$$\begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

are in $\mathcal{A}(R, S)$, while their images under f are

$$\begin{bmatrix} 2 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{bmatrix} \text{ and } \begin{bmatrix} 2 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

Proposition 4.3. If $S = e$, or $S \in \{n - 1, n\}^p$, then $\#\mathcal{F}(R, S) = 1$.

Proof. If S is a vector of all ones and $B \in \mathcal{A}(R, S)$ every column in B must contain only one nonzero element. Then an interchange must also be a column permutation.

If $S \in \{n - 1, n\}^p$ and $B \in \mathcal{A}(R, S)$, the columns in B corresponding to $S_i = n$ must be identically equal to 1, and hence cannot be involved in any interchanges. Then any interchange is between two columns containing $n - 1$ ones, and this can also be represented as a column permutation. \square

Proposition 4.4. If S is strictly decreasing, $\#\mathcal{F}(R, S) = 1$ if and only if $S = R^*$.

Proof. First, we note that $\#\mathcal{F}(R, R^*) = 1$ (as $\#\mathcal{A}(R, R^*) = 1$), so we need to prove the other implication. Let S be strictly decreasing and $\#\mathcal{F}(R, S) = 1$.

Choose $j > i$, so $S_i > S_j$, let $B \in \mathcal{A}(R, S)$ and let b_i and b_j be the i -th and j -th columns of B , respectively. Then $\text{supp } b_j \subseteq \text{supp } b_i$. Otherwise, $\text{supp } b_j \setminus \text{supp } b_i$ contains at least one index, while $\text{supp } b_i \setminus \text{supp } b_j$ contains at least two indices (using $S_i > S_j$), and therefore B satisfies (5). It follows that $\text{supp } b_{i+1} \subseteq \text{supp } b_i$ for all i , and, as R is nonincreasing, all the ones in column i must appear consecutively in the first S_i rows. Hence, by construction, B is equal to the unique matrix in $\mathcal{A}(R, R^*)$ and $S = R^*$. \square

We now consider a special case, in which both $R = S = 2e$ (so $p = n$). The class $\mathcal{A}(R, S)$ is in this case denoted by $\mathcal{A}(n, 2)$ (again, see [4]), and we define $\mathcal{F}(n, 2) = f(\mathcal{A}(n, 2))$.

We can think of a matrix $B \in \mathcal{A}(n, 2)$ as the vertex-edge incidence matrix of a graph. Then we see that the corresponding graph is a union of disjoint cycles (some of which may be cycles on two vertices, so we allow multiple edges in this special case). After a row permutation we may assume there is a sequence of integers $k = (k_1, k_2, \dots, k_t)$ such that the first cycle involves the first k_1 vertices, the next cycle involves the next k_2

and so on. Also, for any such sequence, we see that there is a vertex-edge-incidence matrix in $\mathcal{A}(n, 2)$. We can write B as the direct sum $B = B_1 \oplus B_2 \oplus \cdots \oplus B_t$ where B_i is the vertex-edge-incidence matrix of a cycle on k_i vertices.

If $A \in \mathcal{F}(n, 2)$, then A is permutationally similar to $A_1 \oplus A_2 \oplus \cdots \oplus A_t$, where $A_j = B_j B_j^T$ and B_j is as in the previous paragraph. We say that a matrix of this form is in *canonical form*. The computation of $\#\mathcal{F}(n, 2)$ is complicated due to permutation similarities. However, we do have the following result.

Theorem 4.5. *The number of matrices in $\mathcal{F}(n, 2)$ on canonical form is bounded by the n -th Fibonacci number.*

Proof. $A_1 \oplus A_2 \oplus \cdots \oplus A_t \in \mathcal{F}(n, 2)$ corresponds to some sequence k , where $k_i \geq 2$ for all i . Let a_n denote the number of such sequences k whose sum is n . We note that $a_1 = 0$ and $a_2 = 1$. Now let $n \geq 3$ be some given integer. Then we can choose k_1 in $\{2, 3, \dots, n-2, n\}$. If we define $a_0 = 1$ we see that any choice of k_1 will provide a total of a_{n-k_1} ways to complete the sequence k , and therefore (using $a_1 = 0$)

$$a_n = \sum_{k_1=2}^n a_{n-k_1} = \sum_{s=0}^{n-2} a_s = a_{n-1} + a_{n-2}.$$

□

Note that, in this argument, we counted some sequences several times. For the precise number of matrices in $\mathcal{F}(n, 2)$ in canonical form one needs to count the number of sequences k with $k_i \geq 2$ for all i , and sum n . This is in fact the sequence denoted by A002865 in the integer sequence database OEIS [12], i.e., the number of partitions of n that do not have 1 as a part.

We conclude with a few open questions: (i) What is $\#\mathcal{F}(n, k)$ for $k > 2$?, (ii) If $A \in \mathcal{F}(R, S)$ we have $S \preceq R^*$ and $S^T S = e^T A e$. Is it true that $A \in \mathcal{F}(R, S')$ for all $S' \preceq R^*$ with $(S')^T (S') = e^T A e$?, (iii) For which R, S is the restriction $f|_{\mathcal{A}(R, S)}$ injective?

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