



ELSEVIER

Available online at www.sciencedirect.com

SCIENCE @ DIRECT®

LINEAR ALGEBRA
AND ITS
APPLICATIONS

Linear Algebra and its Applications 363 (2003) 161–176

www.elsevier.com/locate/laa

CP rank of completely positive matrices of order 5

Raphael Loewy^{a,1}, Bit-Shun Tam^{b,*,2}

^aDepartment of Mathematics, Technion, Haifa 32000, Israel

^bDepartment of Mathematics, Tamkang University, Tamsui 25137, Taiwan, ROC

Received 31 October 2000; accepted 6 November 2001

Submitted by J.J. McDonald

Abstract

J.H. Drew et al. [Linear and Multilinear Algebra 37 (1994) 304] conjectured that for $n \geq 4$, the completely positive (CP) rank of every $n \times n$ completely positive matrix is at most $\lceil n^2/4 \rceil$. In this paper we prove that the CP rank of a 5×5 completely positive matrix which has at least one zero entry is at most 6, thus providing new supporting evidence for the conjecture. © 2002 Elsevier Science Inc. All rights reserved.

AMS classification: 15A23; 15A48

Keywords: Completely positive matrix; CP rank; Doubly nonnegative matrix

1. Introduction

An $n \times n$ real symmetric matrix A is called *completely positive* (CP) if A can be represented as BB^t for some $n \times m$ (entrywise) nonnegative matrix B , where B^t denotes the transpose of B . We write $A \in \text{CP}$, or CP_n if it is necessary to indicate the size of A . Clearly a necessary condition for A to be completely positive is that A is nonnegative and (symmetric) positive semidefinite. Such a matrix is called *doubly*

* Corresponding author. Tel.: +886-2-26215656; fax: +886-2-26209916.

E-mail addresses: loewy@techunix.technion.ac.il (R. Loewy), bsm01@mail.tku.edu.tw (B.-S. Tam).

¹ The research of this author was supported by the fund for the promotion of research at the Technion.

² The research of this author was partially supported by the National Science Council of the Republic of China.

nonnegative (DNN), and we write $A \in \text{DNN}$ or DNN_n . For surveys on completely positive matrices we refer the reader to [1–3] and [6, pp. 304–306].

The definition of complete positivity may be alternatively written as

$$A = b_1 b_1^t + \cdots + b_m b_m^t, \quad (1.1)$$

where $b_i \in \mathbb{R}^n$ is nonnegative, $i = 1, \dots, m$.

The b_i 's correspond to the columns of B in the original definition. We refer to this as a *rank 1 CP representation* of A . The latter definition makes it clear that the set CP_n is a convex cone generated by $n \times n$ rank 1 DNN matrices. Either the rank 1 CP representation or the original definition suggests the natural question of determining the minimum value of m in a BB^t representation (or the corresponding rank 1 representation) of a given $A \in \text{CP}$. We denote this number by $\#(A)$, and following Ando [1], we refer to it as the *completely positive rank* or simply the CP rank of A . We note that $\#(A)$ has been previously called the “factorization index” of A by some authors (see, for instance, [2]).

Below are the two well-known major open problems in this area:

1. Determine which doubly nonnegative matrices are completely positive.
2. Given a completely positive matrix A , estimate $\#(A)$.

Much work has been done towards these problems. In particular, in relation to problem (2), Drew et al. [10] posed the following.

Conjecture. If $A \in \text{CP}_n$, $n \geq 4$, then $\#(A) \leq \lfloor n^2/4 \rfloor$.

As evidence for the conjecture, they proved in [10, Corollary 8] that if $A \in \text{CP}_n$, $n \geq 4$, has a triangle-free graph, then $\#(A) \leq \lfloor n^2/4 \rfloor$.

Here by a *graph* G we mean an undirected simple graph. If A is an $n \times n$ symmetric matrix, then by the *graph of* A , denoted by $G(A)$, we mean as usual the graph on vertices $1, 2, \dots, n$, in which there is an edge $\{i, j\}$ if and only if $i \neq j$ and $a_{ij} \neq 0$. We assume the reader is familiar with graph theoretic terminology, which may be found in any standard reference. A graph is said to be *triangle-free* if it contains no triangles. Note that many graphs, such as cycles, trees and bipartite graphs, are triangle-free.

In [10, p. 309] it is also noted that for each $n \geq 4$, the upper bound $\lfloor n^2/4 \rfloor$ can be attained by $\#(A)$ if we choose an $A \in \text{CP}_n$ for which $G(A)$ is complete bipartite with the two parts as balanced as possible.

Two years later, in [9, Theorem 2] Drew and Johnson showed that the conjecture is true for every CP matrix whose graph is a completely positive graph.

A graph G is said to be *completely positive* if every doubly nonnegative matrix A for which $G(A) = G$ is completely positive. The following complete characteriza-

tion of completely positive graphs was achieved in a series of papers [3–5,17]. See also [1,9] for other proofs.

Theorem A. *A graph G is completely positive if and only if it does not contain an odd cycle of length greater than 4.*

More recently, Berman and Shaked-Monderer [7, Theorem 2.1] proved that the conjecture is also true for every $A \in \text{CP}$ for which the comparison matrix $M(A)$ is an M -matrix. In Proposition 1.5 of the same paper, they also provided three other conditions on a symmetric nonnegative matrix A , all equivalent to $M(A)$ being an M -matrix.

An $n \times n$ matrix A is called an M -matrix if A can be written as $\alpha I_n - P$, where P is an $n \times n$ nonnegative matrix and $\alpha \geq \rho(P)$, the spectral radius of P . For a general $n \times n$ matrix A , the *comparison matrix* of $A = (a_{ij})$, denoted by $M(A)$, is defined by

$$M(A)_{ij} = \begin{cases} |a_{ij}| & \text{if } i = j, \\ -|a_{ij}| & \text{if } i \neq j. \end{cases}$$

It is also worthwhile to mention the following two related results obtained in [10, Theorems 5 and 6], which led to [10, Corollary 8] (an affirmative answer to the conjecture for the triangle-free graph case) and also partly motivated the work of Berman and Shaked-Monderer [7].

Theorem B. *If A is a symmetric nonnegative matrix and $G(A)$ is triangle-free, then A is CP if and only if $M(A)$ is an M -matrix.*

Theorem C. *If A is a symmetric nonnegative matrix, $G(A)$ is connected and $M(A)$ is an M -matrix, then $A \in \text{CP}$ and*

$$\#(A) \leq \max \{ |V(G(A))|, |E(G(A))| \},$$

where $E(G(A))$ (respectively, $V(G(A))$) denotes the edge set (respectively, vertex set) of $G(A)$, and for a set S we use $|S|$ to denote its cardinality.

In this paper we shall obtain the following main result, as new supporting evidence for the conjecture.

Theorem. *If $A \in \text{CP}_5$ has at least one zero entry, then $\#(A) \leq 6$.*

Certainly, this paper (likewise, the above-mentioned papers on the conjecture) relies on the earlier work of [8,11,15,18], etc., dealing with the cases $n = 2, 3, 4$. For convenience, we collect some of the relevant results below.

Theorem D.

- (a) For $n \leq 4$, if $A \in \text{DNN}_n$ then $A \in \text{CP}_n$, and in this case $\#(A) \leq n$.
 (b) If $A \in \text{CP}_n$, then $\#(A) = \text{rank } A$, whenever one of the following holds:
 (i) $n = 1, 2$ or 3 ;
 (ii) $\text{rank } A \leq 2$;
 (iii) $n = 4$ and $\text{rank } A = 1, 2$ or 4 .

If it were true that every 5×5 doubly nonnegative matrix was completely positive, then by applying a suitable congruence (see our Lemma 1), we could reduce a 5×5 completely positive matrix all of whose entries are nonzero to a doubly nonnegative, and hence a completely positive, matrix with at least one zero entry. Then by our main theorem (and Observation 2), it would follow that the conjecture was true for all $A \in \text{CP}_5$. Unfortunately, for $n \geq 5$, it was shown by Hall [12] that not every $n \times n$ doubly nonnegative matrix is completely positive. (For other counterexamples, see [1,11,14] and [5] or [10].) So we have not yet fully verified the conjecture when $n = 5$.

2. Auxiliary results

Let $A = (a_{ij}) \in \text{CP}_5$. We want to prove that if A has at least one zero entry, then $\#(A) \leq 6$. Since the property of being CP and also the CP rank are both invariant under permutation similarity, we may assume hereafter that $a_{12} = 0$.

We denote by \mathbb{R}_+^n the set of all nonnegative vectors of \mathbb{R}^n .

We start with any rank 1 CP representation of A , say, $A = \sum_{j=1}^m b_j b_j^t$, where $b_j \in \mathbb{R}_+^5$, $j = 1, \dots, m$. Note that for each j , $1 \leq j \leq m$, either the first or the second component of b_j is zero. Let $A_1 = \{j: \text{the second component of } b_j \text{ is } 0\}$, and let $A_2 = \{1, 2, \dots, m\} \setminus A_1$. Also let $A_1 = \sum_{j \in A_1} b_j b_j^t$ and $A_2 = \sum_{j \in A_2} b_j b_j^t$. Then we obtain a decomposition of A :

$$A = A_1 + A_2, \text{ where } A_i \text{ is CP, } i = 1, 2, \text{ and the second} \quad (2.1)$$

(respectively, first) row of A_1 (respectively, A_2) is zero.

Since the second row and column of A_1 are zero, A_1 is permutationally similar to the direct sum of a 4×4 CP matrix and the 1×1 zero matrix. But the CP rank of a 4×4 CP matrix is at most 4, so it follows that we have $\#(A_1) \leq 4$. For a similar reason, we also have $\#(A_2) \leq 4$. Thus, by a simple argument we have $\#(A) \leq 8$, but this is still far from our target.

We shall make use of the following observations.

By the *support* of a vector x , denoted by $\text{supp}(x)$, we mean the set of indices associated with the nonzero components of x .

Observation 1. Let $u, v \in \mathbb{R}_+^n$. If $\text{supp}(v) \subseteq \text{supp}(u)$, then there exist $\tilde{u}, \tilde{v} \in \mathbb{R}_+^n$, satisfying $uu^t + vv^t = \tilde{u}\tilde{u}^t + \tilde{v}\tilde{v}^t$, such that $\text{supp}(u) = \text{supp}(\tilde{u})$, and for some per-

mutation matrix P , the vectors Pu , $P\tilde{u}$, Pv and $P\tilde{v}$ can be partitioned identically so that they have the following sign patterns:

$$Pu = \begin{bmatrix} + \\ \cdot \\ \cdot \\ \cdot \\ + \\ + \\ \vdots \\ + \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad Pv = \begin{bmatrix} + \\ \cdot \\ \cdot \\ \cdot \\ + \\ 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad P\tilde{u} = \begin{bmatrix} + \\ \cdot \\ \cdot \\ \cdot \\ + \\ + \\ \vdots \\ + \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \text{and } P\tilde{v} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ + \\ \vdots \\ + \\ + \\ \vdots \\ + \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

where the third group (in the partition) may be empty, the second group is empty if $\text{supp}(u) = \text{supp}(v)$, and the first group of $P\tilde{v}$ has at least one 0 and may contain all 0's.

This can be done by applying a procedure, which first appeared in [13, Proof of Lemma 16.2.1], in the context of a completely positive quadratic form for the special case when u and v have the same support. We shall refer to it as the *generalized Hall procedure*, or simply the *GH procedure*.

Suppose $u = (u_1, \dots, u_n)^t$ and $v = (v_1, \dots, v_n)^t$. Then for any real number θ , we have

$$uu^t + vv^t = \begin{bmatrix} u_1 & v_1 \\ u_2 & v_2 \\ \vdots & \vdots \\ u_n & v_n \end{bmatrix} R_\theta^t R_\theta \begin{bmatrix} u_1 & u_2 & \cdots & u_n \\ v_1 & v_2 & \cdots & v_n \end{bmatrix},$$

where R_θ denotes the rotation matrix

$$\begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}.$$

Since $\text{supp}(v) \subseteq \text{supp}(u)$, each of the vectors $(u_1, v_1)^t, \dots, (u_n, v_n)^t$ is of one of the following forms $(+, +)^t, (+, 0)^t$ or $(0, 0)^t$. The action of R_θ on these vectors is to rotate all of them counterclockwise by the same angle θ . (In case $\text{supp}(u) = \text{supp}(v)$, we may also use a clockwise rotation.) We increase θ from zero gradually until it first happens that one (or more) of the vectors of the form $(+, +)^t$ becomes one of the forms $(0, +)^t$. Then the resulting vectors all remain nonnegative, and vectors of the form $(+, 0)^t$ now take the form $(+, +)^t$. Denote the corresponding value of θ by θ_0 , and let $\tilde{u} = (\tilde{u}_1, \dots, \tilde{u}_n)^t$ and $\tilde{v} = (\tilde{v}_1, \dots, \tilde{v}_n)^t$ be the vectors given by

$$R_{\theta_0} \begin{bmatrix} u_1 & u_2 & \cdots & u_n \\ v_1 & v_2 & \cdots & v_n \end{bmatrix} = \begin{bmatrix} \tilde{v}_1 & \tilde{v}_2 & \cdots & \tilde{v}_n \\ \tilde{u}_1 & \tilde{u}_2 & \cdots & \tilde{u}_n \end{bmatrix}.$$

It is easy to check that we have $uu^t + vv^t = \tilde{u}\tilde{u}^t + \tilde{v}\tilde{v}^t$, and the vectors \tilde{u}, \tilde{v} have the desired sign patterns.

Observation 2. Let $A \in \mathbb{C}P_n$ and let $S \in \mathbb{R}^{n,n}$ be such that S is invertible and $S^{-1} \geq 0$. Let $B = SAS^t$. Then, if $B \in \mathbb{C}P_n$ we have $\#(A) \leq \#(B)$.

This is, of course, an obvious known observation (in which it suffices to assume $A \in \mathbb{R}^{n,n}$). It will be used several times in this paper. As in [1, Proof of Theorem 2.6] we shall use S that describes an elementary operation, or more precisely S will have the form $S = I_n - aE_{ij}$, where $a > 0, i \neq j$, and E_{ij} denotes the $n \times n$ matrix with 1 at its (i, j) position and 0 elsewhere. It is easy to see that for such S, S^{-1} exists and is nonnegative.

Observation 3. Let $A = (a_{ij}) \in \mathbb{C}P_5$ be such that $a_{12} = 0$. Consider a decomposition of A as given by (2.1). Suppose that for some $i, 3 \leq i \leq 5$, and some $a > 0$, the matrix $S = I_5 - aE_{i2}$ satisfies $SA_2S^t \in \mathbb{C}P_5$. Then $SAS^t \in \mathbb{C}P_5$. (If we replace E_{i2} and A_2 , respectively, by E_{i1} and A_1 , the assertion still holds.)

This is in fact quite obvious. The congruence we perform amounts to multiplying row 2 by $-a$ and adding it to row i , and doing the corresponding column operation. This does not change A_1 at all, so we have $SAS^t = SA_1S^t + SA_2S^t = A_1 + SA_2S^t$. Thus, SAS^t is a sum of two matrices in $\mathbb{C}P_5$.

We shall also need the following lemmas.

Lemma 1. Let $B = (b_{ij}) \in \text{DNN}_n, n \geq 2$. Suppose that for some $r \neq s, 1 \leq r, s \leq n$, the support of row r is nonempty and is a subset of the support of row s . Then there exists $\alpha > 0$ such that for $S = I_n - \alpha E_{sr}, \tilde{B} = SBS^t \in \text{DNN}_n$ and has the property that the support of its row s is a proper subset of that of the corresponding row of B .

Proof. Without loss of generality, we may assume that $r = 1$ and $s = 2$. Choose $\alpha = \min\{b_{2j}/b_{1j} : b_{1j} > 0\}$. Clearly $\alpha > 0$. Straightforward calculations yield

$$\tilde{B} = SBS^t = \begin{bmatrix} b_{11} & b_{12} - \alpha b_{11} & b_{13} & \cdots & b_{1n} \\ b_{12} - \alpha b_{11} & \tilde{b}_{22} & b_{23} - \alpha b_{13} & \cdots & b_{2n} - \alpha b_{1n} \\ b_{13} & b_{23} - \alpha b_{13} & b_{33} & \cdots & b_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{1n} & b_{2n} - \alpha b_{1n} & b_{3n} & \cdots & b_{nn} \end{bmatrix},$$

where $\tilde{b}_{22} = b_{22} - \alpha b_{12} - \alpha(b_{12} - \alpha b_{11})$. It is clear that \tilde{B} is positive semidefinite, and so we have $\tilde{b}_{22} \geq 0$. By our choice of α , it is also clear that the remaining entries

of \tilde{B} are all nonnegative. Therefore, \tilde{B} is DNN. It remains to show that the support of row 2 of \tilde{B} has the desired properties. In view of our assumptions on rows 1 and 2 of the DNN matrix B , clearly the numbers b_{11} , $b_{21} (= b_{12})$ and b_{22} are all positive. The positive semidefiniteness of B also implies that we have $\det B[\{1, 2\}] \geq 0$, and hence $b_{22}/b_{12} \geq b_{12}/b_{11}$. So, the minimum value α of the set $\{b_{2j}/b_{1j} : b_{1j} > 0\}$ can be attained for some $j \neq 2$. Now it should be clear that the support of row 2 of \tilde{B} is a proper subset of that of the corresponding row of B . \square

The following lemma can be deduced from [5, Theorem 4.1]. Here we offer an independent, self-contained proof.

Lemma 2. *Let*

$$P = \begin{bmatrix} p_{11} & p_{12} & p_{13} & p_{14} \\ p_{12} & p_{22} & 0 & 0 \\ p_{13} & 0 & p_{33} & p_{34} \\ p_{14} & 0 & p_{34} & p_{44} \end{bmatrix}$$

be a rank 3 DNN matrix with $p_{12} > 0$. Then $\#(P) = 3$.

Proof. By a known result, we have $P \in \text{CP}_4$ and $\#(P) \geq \text{rank } P = 3$. We multiply the second row of P by $-p_{12}/p_{22}$ and add it to the first row, and do the corresponding column operation. We get the matrix

$$\tilde{P} = \begin{bmatrix} p_{11} - (p_{12}^2/p_{22}) & 0 & p_{13} & p_{14} \\ 0 & p_{22} & 0 & 0 \\ p_{13} & 0 & p_{33} & p_{34} \\ p_{14} & 0 & p_{34} & p_{44} \end{bmatrix}$$

which is clearly a rank 3, DNN and hence CP matrix. By Observation 2 we have $\#(P) \leq \#(\tilde{P})$. Since $p_{22} > 0$ (as P is positive semidefinite and $p_{12} > 0$), it follows that $\tilde{P}[\{1, 3, 4\}]$ is a rank 2 CP matrix, so its CP rank is 2. Hence $\#(\tilde{P}) = 3$, implying $\#(P) = 3$. \square

3. Proof of the main result

To prove our theorem, we start with the decomposition (2.1), and use Observation 3 repeatedly and systematically to obtain more 0's in the (transformed) matrices A_1 and A_2 . In view of Observation 2, if we can show at the end of this process that the transformed matrix A has CP rank 6 or less, then so does the original A .

For convenience, to avoid complications in the notation, we *do not change the names* of A, A_1, A_2 at each transformation we perform.

We let \hat{A}_1 denote the 4×4 matrix obtained from A_1 by deleting its second row and column (which are zero), and let \hat{A}_2 denote the 4×4 matrix obtained from A_2 by deleting its first row and column (which are zero). Clearly, we have $\hat{A}_1, \hat{A}_2 \in \text{CP}_4$.

We now use Observation 3, in conjunction with Lemma 1. We work first with A_2 , or more precisely \hat{A}_2 , and try to get as many 0's as possible in the transformed matrix. Denote the (i, j) entry of \hat{A}_2 by \hat{a}_{ij} . Note that if $\hat{a}_{11} = 0$ then the first row and column of \hat{A}_2 are zero, and it follows that the second row and column of A are zero; in which case clearly we have $\#(A) \leq 4$. So, henceforth, we assume that $\hat{a}_{11} > 0$.

We may assume that \hat{A}_2 has already a zero in its second row. Otherwise, apply Lemma 1 (with $r = 1$ and $s = 2$) to get a zero there.

We consider two cases.

Case I: Suppose that $\hat{a}_{21} (= \hat{a}_{12}) = 0$; that is,

$$\hat{A}_2 = \begin{bmatrix} + & 0 & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix},$$

where \cdot for an entry of a matrix means it can be zero or positive.

(Ia) Suppose $\hat{a}_{13} = \hat{a}_{14} = 0$, so

$$\hat{A}_2 = \left[\begin{array}{c|ccc} + & 0 & 0 & 0 \\ 0 & & & \\ \hline 0 & & A_3 & \\ 0 & & & \end{array} \right], \quad \text{where } A_3 \in \text{CP}_3.$$

Then

$$A = \begin{bmatrix} \cdot & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 \\ \cdot & 0 & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & & & \\ 0 & 0 & A_3 & & \\ 0 & 0 & & & \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & + & 0 & 0 & 0 \\ 0 & 0 & & & \\ 0 & 0 & & 0 & \\ 0 & 0 & & & \end{bmatrix}.$$

Clearly, the sum of the first two terms is a CP matrix with CP rank ≤ 4 . So we have $\#(A) \leq 5$.

(Ib) Suppose exactly one of $\hat{a}_{13}, \hat{a}_{14}$ is 0. By symmetry, we may assume $\hat{a}_{13} = 0$, that is,

$$\hat{A}_2 = \begin{bmatrix} + & 0 & 0 & + \\ 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot \\ + & \cdot & \cdot & + \end{bmatrix}.$$

Since the support of row 1 of \hat{A}_2 is included in that of its row 4, by Lemma 1 we can use an allowable congruence that annihilates the $(4, 1)$ and $(1, 4)$ entries. (If it happens that the $(4, 4)$ entry is annihilated, then by the positive semidefiniteness of the transformed \hat{A}_2 , the $(4, 1)$ and $(1, 4)$ entries also become zero.) So we are back to (Ia) and in view of Observation 2 we have $\#(A) \leq 5$.

(Ic) Suppose $\hat{a}_{13} > 0$ and $\hat{a}_{14} > 0$; that is,

$$\hat{A}_2 = \begin{bmatrix} + & 0 & + & + \\ 0 & \cdot & \cdot & \cdot \\ + & \cdot & + & \cdot \\ + & \cdot & \cdot & + \end{bmatrix}.$$

If we also have $\hat{a}_{34} > 0$, then by Lemma 1 we can use an allowable congruence to annihilate either \hat{a}_{31} (and \hat{a}_{13}) or \hat{a}_{34} (and \hat{a}_{43}). If we get the 0 in the (3, 1) position, we are back to (Ib) and we are done. So we may assume that $\hat{a}_{34} = \hat{a}_{43} = 0$; that is,

$$\hat{A}_2 = \begin{bmatrix} + & 0 & + & + \\ 0 & \cdot & \cdot & \cdot \\ + & \cdot & + & 0 \\ + & \cdot & 0 & + \end{bmatrix}.$$

We now write a rank 1 CP representation of \hat{A}_2 ; that is, its representation as a sum of matrices of the form xx^t , where $x \in \mathbb{R}_+^4$. We know we may assume that the number of summands is ≤ 4 . Also, when we go back to A_2 itself, all we need to do is to take each such vector x and add a 0 component as the first component. In view of the sign pattern of \hat{A}_2 , it is clear that if x is any such vector, then

$$x_1x_2 = 0 \quad \text{and} \quad x_3x_4 = 0. \tag{3.1}$$

We divide these vectors x into two groups. The first group is composed of vectors with positive first component, whereas the second group is composed of vectors with zero first component. Let l denote the number of vectors in the first group. Note that each summand in the rank 1 CP representation of A_2 (corresponding to the said representation of \hat{A}_2) that comes from a vector of the second group can be removed and added to A_1 . If $l \leq 2$, we are done, as we know $\#(A_1) \leq 4$. So we consider the case $l \geq 3$. In view of (3.1), the following are the possible sign patterns for vectors of the first type:

$$\begin{matrix} \begin{bmatrix} + \\ 0 \\ 0 \\ 0 \end{bmatrix}, & \begin{bmatrix} + \\ 0 \\ + \\ 0 \end{bmatrix}, & \begin{bmatrix} + \\ 0 \\ 0 \\ + \end{bmatrix}. \\ \text{(i)} & \text{(ii)} & \text{(iii)} \end{matrix}$$

Clearly it suffices to have at most one vector with pattern (i). We claim that the same is true for patterns (ii) and (iii). Indeed consider (ii), for example, because (iii) can be done similarly.

By applying Observation 1 or the *GH* procedure (with u and v interchanged or using a clockwise rotation, if necessary), we may replace any two vectors with patterns

$$\begin{bmatrix} + \\ 0 \\ + \\ 0 \end{bmatrix}, \begin{bmatrix} + \\ 0 \\ + \\ 0 \end{bmatrix}$$

(which, we may assume, are linearly independent) by two vectors with patterns

$$\begin{bmatrix} + \\ 0 \\ + \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ + \\ 0 \end{bmatrix},$$

and then we can move the second vector to the second group.

Thus, we can assume that there is at most one vector with any one of the patterns (i), (ii) or (iii). We can assume further that there is *exactly* one vector of each pattern, or else $l \leq 2$ and we are done. Now we can apply the *GH* procedure again to

$$\begin{bmatrix} + \\ 0 \\ + \\ 0 \end{bmatrix}, \begin{bmatrix} + \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

to get

$$\begin{bmatrix} + \\ 0 \\ + \\ 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 \\ 0 \\ + \\ 0 \end{bmatrix},$$

and again we can move one summand to A_1 . Thus, the case $l \geq 3$ reduces to the case $l \leq 2$ and we conclude that $\#(A) \leq 6$.

This concludes the proof of Case I. The argument of Case I also shows that if the (3, 1) or (4, 1) entry is zero for \hat{A}_2 or for an intermediate \hat{A}_2 , we are also done.

Case II: Suppose that $\hat{a}_{21}, \hat{a}_{31}, \hat{a}_{41}$ (and hence also $\hat{a}_{22}, \hat{a}_{33}, \hat{a}_{44}$) are all positive.

Then we can assume $\hat{a}_{23} = 0$ or $\hat{a}_{24} = 0$; otherwise, apply Lemma 1 to rows 1 and 2 of \hat{A}_2 . By symmetry, we can assume $\hat{a}_{23} = 0$. So

$$\hat{A}_2 = \begin{bmatrix} + & + & + & + \\ + & + & 0 & \cdot \\ + & 0 & + & \cdot \\ + & \cdot & \cdot & + \end{bmatrix}.$$

If the entries in row 4 of \hat{A}_2 are all nonzero, we apply Lemma 1 to rows 1 and 4 to obtain a zero there. If $\hat{a}_{41} = 0 = \hat{a}_{14}$, then as noted at the end of the proof of Case I, we are done. So assume $\hat{a}_{41} > 0$. Then $\hat{a}_{42} = 0$ or $\hat{a}_{43} = 0$. By symmetry we can assume $\hat{a}_{42} = 0$; otherwise permute rows 2 and 3, and the corresponding columns, noting that this does not change the 0 in the (2, 3) and (3, 2) positions. So we have

$$\hat{A}_2 = \begin{bmatrix} + & + & + & + \\ + & + & 0 & 0 \\ + & 0 & + & \cdot \\ + & 0 & \cdot & + \end{bmatrix},$$

and therefore

$$A_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & + & + & + & + \\ 0 & + & + & 0 & 0 \\ 0 & + & 0 & + & \cdot \\ 0 & + & 0 & \cdot & + \end{bmatrix}. \tag{3.2}$$

Note that the situation described by (3.2) is the only one where we have *not* proved our claim. But we have the extra information that the graph $G(A_2)$ misses the edges $\{3, 4\}$ and $\{3, 5\}$. Since we might have used permutations, we can say that if we cannot finish the proof using our work with A_2 alone, then the graph $G(A_2)$ misses at least two of the edges $\{3, 4\}$, $\{3, 5\}$, and $\{4, 5\}$.

But now we can work in a similar way with \hat{A}_1 . It is clear from the proof so far, and in particular from the previous paragraph, that we get the desired result *unless* the graphs $G(A_1)$ and $G(A_2)$ both miss at least two of the edges $\{3, 4\}$, $\{3, 5\}$, $\{4, 5\}$, and $G(A_1)$ contains the edges $\{1, 3\}$, $\{1, 4\}$, $\{1, 5\}$, and $G(A_2)$ contains the edges $\{2, 3\}$, $\{2, 4\}$, and $\{2, 5\}$. Applying a suitable permutation similarity to A (and hence also to A_1 and A_2 simultaneously), hereafter we may assume that A_2 is given by (3.2) and the $(3, 4)$ entry of A_1 is zero.

We have to consider two cases.

Case (a):

$$A_1 = \begin{bmatrix} + & 0 & + & + & + \\ 0 & 0 & 0 & 0 & 0 \\ + & 0 & + & 0 & 0 \\ + & 0 & 0 & + & \cdot \\ + & 0 & 0 & \cdot & + \end{bmatrix}.$$

This and (3.2) imply $a_{12} = a_{34} = a_{35} = 0$.

Consider a rank 1 CP representation of A . We divide the nonnegative vectors that are involved in this representation into two groups. The first group consists of vectors with positive third component, whereas the second group consists of vectors with zero third component. Suppose that y is a vector in the first group, so $y_3 > 0$. Then we must have

$$y_1 y_2 = 0 \quad \text{and} \quad y_4 = y_5 = 0.$$

The only possible sign patterns for vectors in this group are therefore

$$\begin{matrix} \begin{bmatrix} 0 \\ 0 \\ + \\ 0 \\ 0 \end{bmatrix}, & \begin{bmatrix} + \\ 0 \\ + \\ 0 \\ 0 \end{bmatrix}, & \begin{bmatrix} 0 \\ + \\ + \\ 0 \\ 0 \end{bmatrix}. \\ \text{(i)} & \text{(ii)} & \text{(iii)} \end{matrix}$$

As in the proof of Case (Ic), using the *GH* procedure and moving certain resulting vectors to the second group, we may assume that in the first group we have at most

one vector of each type. If we have exactly one vector of each type, we apply the *GH* procedure to

$$\begin{bmatrix} 0 \\ 0 \\ + \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} + \\ 0 \\ + \\ 0 \\ 0 \end{bmatrix}$$

to get

$$\begin{bmatrix} + \\ 0 \\ + \\ 0 \\ 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} + \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

and we can move the second vector to the second group. So, in any case, at the end of this process we are left with at most two vectors in the first group, possibly increasing the number of vectors in the second group. But the sum of rank 1 matrices corresponding to vectors in the second group is a 5×5 CP matrix whose third row and column vanish, so its CP rank is ≤ 4 . Hence $\#(A) \leq 6$.

Case (b):

$$A_1 = \begin{bmatrix} + & 0 & + & + & + \\ 0 & 0 & 0 & 0 & 0 \\ + & 0 & + & 0 & + \\ + & 0 & 0 & + & 0 \\ + & 0 & + & 0 & + \end{bmatrix}.$$

For simplicity, we write $B = A_2$ and $C = A_1$, so

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & b_{22} & b_{23} & b_{24} & b_{25} \\ 0 & b_{23} & b_{33} & 0 & 0 \\ 0 & b_{24} & 0 & b_{44} & b_{45} \\ 0 & b_{25} & 0 & b_{45} & b_{55} \end{bmatrix}, \quad (3.3)$$

$$C = \begin{bmatrix} c_{11} & 0 & c_{13} & c_{14} & c_{15} \\ 0 & 0 & 0 & 0 & 0 \\ c_{13} & 0 & c_{33} & 0 & c_{35} \\ c_{14} & 0 & 0 & c_{44} & 0 \\ c_{15} & 0 & c_{35} & 0 & c_{55} \end{bmatrix}.$$

By (3.2), b_{22} , b_{23} , b_{24} , b_{25} , b_{33} , b_{44} , and b_{55} are all positive. We can also assume $b_{45} > 0$, or else we have $a_{45} = 0$ (and $a_{12} = 0$, $a_{43} = 0$), so we can handle it like Case (a).

If $B[\{2, 3, 4, 5\}]$ and $C[\{1, 3, 4, 5\}]$ are both singular, then by Lemma 2 we are done. So we can assume that at least one of these matrices is positive definite. By symmetry, we may assume $B[\{2, 3, 4, 5\}]$ is positive definite.

We perform one additional normalization. We may apply a congruence by a diagonal matrix with positive diagonal entries to get

$$b_{44} = b_{45}.$$

So we assume from now on that this equality holds, and as a consequence we also have

$$b_{44} < b_{55}.$$

Then one can easily see that, for any $0 \leq \alpha < b_{44}$, the matrix

$$\begin{bmatrix} b_{44} - \alpha & b_{44} - \alpha \\ b_{44} - \alpha & b_{55} - \alpha \end{bmatrix}$$

is positive definite and nonnegative.

Let α and β be real indeterminates and define

$$B(\alpha, \beta) = \begin{bmatrix} b_{22} & b_{23} & b_{24} & b_{25} \\ b_{23} & b_{33} + \beta & 0 & 0 \\ b_{24} & 0 & b_{44} - \alpha & b_{44} - \alpha \\ b_{25} & 0 & b_{44} - \alpha & b_{55} - \alpha \end{bmatrix},$$

$$C(\alpha, \beta) = \begin{bmatrix} c_{11} & c_{13} & c_{14} & c_{15} \\ c_{13} & c_{33} - \beta & 0 & c_{35} \\ c_{14} & 0 & c_{44} + \alpha & \alpha \\ c_{15} & c_{35} & \alpha & c_{55} + \alpha \end{bmatrix}.$$

So $B[\{2, 3, 4, 5\}] = B(0, 0)$ and $C[\{1, 3, 4, 5\}] = C(0, 0)$. Define

$$T = \{(\alpha, \beta) : \alpha, \beta \geq 0, B(\alpha, \beta), C(\alpha, \beta) \in \text{DNN and } B(\alpha, \beta) \text{ is singular}\}.$$

We claim that T is a nonempty set. To show this, observe that $B(0, 0)$ is a positive definite and nonnegative matrix, while $B(b_{44}, 0)$ is a nonnegative matrix which is not positive semidefinite. Hence, there exists $\alpha_0, 0 < \alpha_0 < b_{44}$, such that $B(\alpha_0, 0)$ is a singular DNN matrix. It is obvious that $C(\alpha_0, 0)$ is a DNN matrix, so $(\alpha_0, 0) \in T$. Note also that T is a bounded set.

Let $T_1 = \{\alpha : \alpha > 0 \text{ and there exists } \beta \geq 0 \text{ such that } (\alpha, \beta) \in T\}$.

Remark 1. It is possible to show that if $\alpha \in T_1$ then there exists a *unique* $\beta \geq 0$ such that $(\alpha, \beta) \in T$. But uniqueness is not required to continue this proof.

Now let

$$\varphi = \sup_{\alpha \in T_1} \alpha.$$

It is clear that φ is well defined, and in fact $\varphi \geq \alpha_0$. Let $\{\alpha_j\}$ be an increasing sequence of elements of T_1 which converges to φ . Let $\{\beta_j\}$ be a sequence of real numbers such that for each j , $(\alpha_j, \beta_j) \in T$. By choosing an appropriate subsequence if necessary, we may assume that the sequence $\{\beta_j\}$ converges to a limit ψ . It follows that the sequences $\{B(\alpha_j, \beta_j)\}$ and $\{C(\alpha_j, \beta_j)\}$ converge, respectively, to $B(\varphi, \psi)$ and $C(\varphi, \psi)$. It is clear that $B(\varphi, \psi)$ and $C(\varphi, \psi)$ are DNN matrices, and $B(\varphi, \psi)$ is singular.

We claim that $C(\varphi, \psi)$ is also singular. Indeed, if this is not the case, then $C(\varphi, \psi)$ is positive definite, and so there exists $\delta > 0$ such that

$$C(\varphi, \psi + \delta) = \begin{bmatrix} c_{11} & c_{13} & c_{14} & c_{15} \\ c_{13} & c_{33} - \psi - \delta & 0 & c_{35} \\ c_{14} & 0 & c_{44} + \varphi & \varphi \\ c_{15} & c_{35} & \varphi & c_{55} + \varphi \end{bmatrix}$$

is a nonnegative and positive definite matrix. In view of

$$\begin{aligned} 0 &= \det B(\varphi, \psi) \\ &= -b_{23} \det \begin{bmatrix} b_{23} & b_{24} & b_{25} \\ 0 & b_{44} - \varphi & b_{44} - \varphi \\ 0 & b_{44} - \varphi & b_{55} - \varphi \end{bmatrix} \\ &\quad + (b_{33} + \psi) \det \begin{bmatrix} b_{22} & b_{24} & b_{25} \\ b_{24} & b_{44} - \varphi & b_{44} - \varphi \\ b_{25} & b_{44} - \varphi & b_{55} - \varphi \end{bmatrix} \\ &= -b_{23}^2 (b_{44} - \varphi)(b_{55} - b_{44}) + (b_{33} + \psi) \det \begin{bmatrix} b_{22} & b_{24} & b_{25} \\ b_{24} & b_{44} - \varphi & b_{44} - \varphi \\ b_{25} & b_{44} - \varphi & b_{55} - \varphi \end{bmatrix}, \end{aligned}$$

it is clear that the positive semidefinite matrix

$$\begin{bmatrix} b_{22} & b_{24} & b_{25} \\ b_{24} & b_{44} - \varphi & b_{44} - \varphi \\ b_{25} & b_{44} - \varphi & b_{55} - \varphi \end{bmatrix}$$

has a positive determinant and hence is positive definite. Then we readily see that the matrix

$$B(\varphi, \psi + \delta) = \begin{bmatrix} b_{22} & b_{23} & b_{24} & b_{25} \\ b_{23} & b_{33} + \psi + \delta & 0 & 0 \\ b_{24} & 0 & b_{44} - \varphi & b_{44} - \varphi \\ b_{25} & 0 & b_{44} - \varphi & b_{55} - \varphi \end{bmatrix}$$

has a positive determinant, and since it contains a positive definite principal submatrix of order 1 less, we conclude that $B(\varphi, \psi + \delta)$ is a nonnegative and positive definite matrix. Moreover, $B(b_{44}, \psi + \delta)$ is a nonnegative matrix which is not positive semidefinite. It follows that there exists $\varepsilon > 0$ such that $B(\varphi + \varepsilon, \psi + \delta)$ is a singular

DNN matrix, and clearly $C(\varphi + \varepsilon, \psi + \delta)$ is a DNN matrix. This contradiction to the definition of φ shows that $C(\varphi, \psi)$ is a singular matrix.

Finally, consider the following decomposition of A :

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & b_{22} & b_{23} & b_{24} & b_{25} \\ 0 & b_{23} & b_{33} + \psi & 0 & 0 \\ 0 & b_{24} & 0 & b_{44} - \varphi & b_{44} - \varphi \\ 0 & b_{25} & 0 & b_{44} - \varphi & b_{55} - \varphi \end{bmatrix} + \begin{bmatrix} c_{11} & 0 & c_{13} & c_{14} & c_{15} \\ 0 & 0 & 0 & 0 & 0 \\ c_{13} & 0 & c_{33} - \psi & 0 & c_{35} \\ c_{14} & 0 & 0 & c_{44} + \varphi & \varphi \\ c_{15} & 0 & c_{35} & \varphi & c_{55} + \varphi \end{bmatrix}.$$

Let us denote the first and second summands by \tilde{B} and \tilde{C} , respectively. By Lemma 2 it is clear that $\#(\tilde{B}) \leq 3$. But we cannot apply Lemma 2 to \tilde{C} . Note that c_{15} , c_{35} and φ are all positive numbers. So, if we delete the second row and column of \tilde{C} , then the resulting matrix \hat{C} has a positive last row and column. Now we can apply Lemma 1 (with $r = 1$ and $s = 4$) to \hat{C} to obtain a 0 in its last row. After the operation, if $\hat{c}_{41} = 0$, then by the argument of Case I (with \tilde{C} and \tilde{B} playing, respectively, the roles of A_2 and A_1 there), we have $\#(A) \leq 6$. On the other hand, if \hat{c}_{42} or $\hat{c}_{43} = 0$, then we can apply Lemma 2 to conclude that $\#(\tilde{C}) \leq 3$. But $\#(\tilde{B}) \leq 3$, so we have $\#(A) \leq 6$. This completes the proof.

References

- [1] T. Ando, Completely Positive Matrices, Lecture Notes, Sapporo, Japan, 1991.
- [2] A. Berman, Complete positivity, Linear Algebra Appl. 107 (1988) 57–63.
- [3] A. Berman, Completely positive graphs, in: Combinatorial and Graph-Theoretical Problems in Linear Algebra, The IMA Volumes in Mathematics and its Applications, vol. 50, Springer, New York, 1993, pp. 229–233.
- [4] A. Berman, R. Grone, Bipartite completely positive matrices, Math. Proc. Cambridge Philos. Soc. 103 (1988) 269–276.
- [5] A. Berman, D. Hershkowitz, Combinatorial results on completely positive matrices, Linear Algebra Appl. 95 (1987) 111–125.
- [6] A. Berman, R.J. Plemmons, Nonnegative Matrices in the Mathematical Sciences, Classics in Applied Mathematics, SIAM, Philadelphia, 1994 (revised reprint of the 1979 original).
- [7] A. Berman, N. Shaked-Monderer, Remarks on completely positive matrices, Linear and Multilinear Algebra 44 (1998) 149–163.
- [8] P.H. Diananda, On non-negative forms in real variables some or all of which are nonnegative, Proc. Cambridge Philos. Soc. 58 (1962) 17–25.
- [9] J.H. Drew, C.R. Johnson, The no long odd cycle theorem for completely positive matrices, in: Random Discrete Structures, The IMA Volumes in Mathematics and its Applications, vol. 76, Springer, New York, 1996, pp. 103–115.

- [10] J.H. Drew, C.R. Johnson, R. Loewy, Completely positive matrices associated with M -matrices, *Linear and Multilinear Algebra* 37 (1994) 303–310.
- [11] L.J. Gray, D.G. Wilson, Nonnegative factorization of positive semidefinite nonnegative matrices, *Linear Algebra Appl.* 31 (1980) 119–127.
- [12] M. Hall Jr., A survey of combinatorial analysis, *Some Aspects of Analysis and Probability, Surveys in Applied Mathematics*, vol. 4, Wiley, New York, 1958, pp. 35–104.
- [13] M. Hall Jr., *Combinatorial Theory*, Blaisdell, Lexington, 1967 (second ed., 1986).
- [14] J. Hannah, T.J. Laffey, Nonnegative factorization of completely positive matrices, *Linear Algebra Appl.* 55 (1983) 1–9.
- [15] M. Hall Jr., M. Newman, Copositive and completely positive quadratic forms, *Proc. Cambridge Philos. Soc.* 59 (1963) 329–339.
- [16] M. Kaykobad, On nonnegative factorization of matrices, *Linear Algebra Appl.* 96 (1987) 27–33.
- [17] N. Kogan, A. Berman, Characterization of completely positive graphs, *Discrete Math.* 114 (1993) 297–304.
- [18] J.E. Maxfield, H. Minc, On the equation $X'X = A$, *Proc. Edinburgh Math. Soc.* 13 (1962) 125–129.