5 × 5 Completely positive matrices
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Abstract
We study the problem of determining whether a given 5 × 5 matrix is completely positive, by investigating the number of negative entries of a Schur complement of A. We show that if this number is not 4, then A is completely positive, and present some sufficient conditions for A to be cp when this number is 4. We also show that the complete positivity of an elementwise positive doubly nonnegative 5 × 5 matrix is equivalent to the complete positivity of a related 5 × 5 doubly nonnegative matrix that is not elementwise positive.

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1. Introduction

A matrix A is completely positive if it can be decomposed as $A = BB^T$, where $B$ is a (not necessarily square) elementwise nonnegative matrix. Clearly, if A is

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completely positive, then it is **doubly nonnegative**, i.e., positive semidefinite and (elementwise) nonnegative (when we refer to a matrix as positive or nonnegative, we will always mean elementwise positive and elementwise nonnegative). This necessary condition is also sufficient for matrices of order \( n \leq 4 \), but not for \( n \geq 5 \), e.g., [8]. Qualitative analysis of when the necessary conditions are sufficient is done in [1,3,4,6]. This is done by associating with an \( n \times n \) real matrix \( A \) a graph \( G(A) \) with vertex set \( V = \{ v_1, v_2, \ldots, v_n \} \) and edge set \( E(G(A)) = \{ \{ v_i, v_j \} | a_{ij} \neq 0, i \neq j \} \). If \( A \) is completely positive, the smallest number of columns of \( B \) such that \( A = BB^T, B \geq 0 \) is called the ‘cp-rank’ of \( A \). For \( n \leq 4 \), \( \text{cp-rank}(A) \leq n \). If \( A \) is a \( 5 \times 5 \) completely positive matrix with some zero entries, then \( \text{cp-rank}(A) \leq 6 \), [7]. A recent reference on applications and properties of completely positive matrices and on ‘cp-rank’ is [5]. We shall use \( \text{cp}, \text{dnn}, \text{psd} \), and \( \text{pd} \) as short notations for completely positive, doubly nonnegative, positive semidefinite and positive definite, and denote by \( \text{CP}_n, \text{DNN}_n, \text{PSD}_n \), and \( \text{PD}_n \), respectively, the sets of all the \( \text{cp}, \text{dnn}, \text{psd}, \text{pd} \) matrices of order \( n \). We also use the notation \( [n] \) for the set \( \{ 1, 2, \ldots, n \} \), \( I_n \) for the identity matrix of order \( n \), and \( R^n_+ \) for the nonnegative orthant of \( R^n \). For an \( n \times n \) matrix \( A \) and \( \alpha \subseteq [n] \), we denote the principal submatrix of \( A \) indexed by \( \alpha \) by \( A(\alpha) \). We also denote \( A[[n]\setminus\alpha] \) by \( A(\alpha) \). We use the notation \( E_{ij} \) for a matrix of all zero entries except in the position \((i, j)\) that is 1.

For any \( n \times n \) matrix \( A \), partitioned in the form

\[
\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix},
\]

where \( A_{11}, A_{22} \) are square, with \( A_{22} \) nonsingular, we denote by \( A/A_{22} \) the Schur complement of \( A_{22} \), i.e., \( A/A_{22} = A_{11} - A_{12}A_{22}^{-1}A_{21} \).

In this paper we give conditions for a \( 5 \times 5 \) dnn matrix to be cp. The case in which \( A \) has at least two zeros above the main diagonal was studied in [9]. Here we first study the case when \( A \) has at least one zero above the diagonal by considering the number of negative entries of the Schur complement \( A/A_{22} \). In Section 2, we present some observations concerning complete positivity of \( A \). In Section 3 we show that if \( a_{45} = 0 \) and the number of negative entries above the main diagonal of the Schur complement \( C = A/A[[4, 5]] \), denoted by \( \mu(C) \), is not 2, then \( A \) is cp. In Section 4 we study in detail the case \( \mu(C) = 2 \), and obtain some sufficient conditions for \( A \) to be cp. In Section 5, we reduce \( A \) to the cases with at least 4 zero entries in the case \( \mu(C) = \text{rank}(C) = 2 \). In Section 6, we show that the complete positivity of a positive dnn \( 5 \times 5 \) matrix is equivalent to the complete positivity of a related \( 5 \times 5 \) dnn matrix which is not positive. We conclude the paper by summarizing the sufficient conditions that we have presented for complete positivity of a given \( 5 \times 5 \) real matrix, and by suggesting conjectures concerning the unsettled cases.
2. Some observations

Let \( A \) be a 5 \times 5 dnn matrix with at least one zero entry above the diagonal. We want to determine if \( A \) is cp. Since both double nonnegativity and complete positivity are not affected by nonnegative scaling, \( A \to DAD \), where \( D \) is a nonnegative diagonal matrix, or by permutation similarity, \( A \to P^TAP \), where \( P \) is a permutation matrix, and since \( a_{ii} = 0 \) implies that both the \( i \)th row and the \( i \)th column are zero, we can assume that

\[
A = \begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix} = \begin{bmatrix}
A_{11} & \alpha_1 & \alpha_2 \\
\alpha_1^T & 1 & 0 \\
\alpha_2^T & 0 & 1
\end{bmatrix},
\]

(2.1)

where \( A_{11} \) is a 3 \times 3 dnn matrix, \( A_{22} \) is a 2 \times 2 identity matrix, \( A_{12} = [\alpha_1, \alpha_2] \), \( A_{21} = A_{12}^T \), and \( \alpha_1, \alpha_2 \in \mathbb{R}_3^+ \).

Throughout the paper we shall assume that \( A \) is a 5 \times 5 dnn matrix in form (2.1).

**Theorem 2.1.** \( A \) is cp if and only if there exist two dnn matrices \( B_1, B_2 \) such that

\[
A_{11} = B_1 + B_2
\]

(2.2)

and

\[
\begin{bmatrix}
B_i \\
\alpha_i \\
\alpha_i^T
\end{bmatrix} \in \text{DNN}_4
\]

(2.3)

for \( i = 1, 2 \).

**Proof.** “If” Let

\[
A_1 = \begin{bmatrix}
B_1 & \alpha_1 & 0 \\
\alpha_1^T & 1 & 0 \\
0 & 0 & 0
\end{bmatrix}
\]

(2.4)

and

\[
A_2 = \begin{bmatrix}
B_2 & 0 & \alpha_2 \\
0 & 0 & 0 \\
\alpha_2^T & 0 & 1
\end{bmatrix}
\]

(2.5)

Then

\[
A_1 = \begin{bmatrix}
B_1 & \alpha_1 \\
\alpha_1^T & 1
\end{bmatrix} \oplus [0],
\]

and \( A_2 \) is permutation similar to

\[
\begin{bmatrix}
B_2 & \alpha_2 \\
\alpha_2^T & 1
\end{bmatrix} \oplus [0].
\]
Since for $n = 4$ complete positivity is equivalent to double nonnegativity, $A_1$ and $A_2$ are cp, and so $A = A_1 + A_2$ is also cp.

"Only if" Suppose $A$ is cp. We have to find $3 \times 3$ dnn matrices $B_1, B_2$ that satisfy (2.2) and (2.3). Since $A$ is cp, there exist $m$ ($\leq 6$, by [7]) nonnegative vectors $b_1, b_2, \ldots, b_m \in \mathbb{R}_+^3$ such that

$$A = b_1 b_1^T + \cdots + b_m b_m^T.$$  

(2.6)

For each $i$ in $[m]$, partition $b_i$ as

$$b_i = \begin{bmatrix} \tilde{b}_i \\ c_i \\ d_i \end{bmatrix},$$

where $\tilde{b}_i \in \mathbb{R}_+^3$, and $c_i, d_i$ are nonnegative numbers.

Since $A_{22} = I_2$, $c_i \neq 0$ for at least one index $i$, $d_i \neq 0$ for at least one index $i$, and $c_i d_i = 0$ for all $i = 1, 2, \ldots, m$; so without loss of generality we may assume that

- $c_i > 0, \quad d_i = 0; \quad i = 1, \ldots, r,$
- $c_i = 0, \quad d_i > 0; \quad i = r + 1, \ldots, p,$
- $c_i = 0, \quad d_i = 0; \quad i = p + 1, \ldots, m,$

where $p$ ($\leq m$) may be equal to $m$. By denoting $B_1 = \sum_{j=1}^r \tilde{b}_j \tilde{b}_j^T$, $B_2 = \sum_{j=r+1}^m \tilde{b}_j \tilde{b}_j^T$, we readily get

$$b_1 b_1^T + \cdots + b_r b_r^T = \begin{bmatrix} B_1 & \alpha_1 & 0 \\ \alpha_1^T & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \in \mathbb{CP}_5$$

and

$$b_{r+1} b_{r+1}^T + \cdots + b_m b_m^T = \begin{bmatrix} B_2 & 0 & \alpha_2 \\ 0 & 0 & 0 \\ \alpha_2^T & 0 & 1 \end{bmatrix} \in \mathbb{CP}_5.$$  

It is easy to check that (2.2) and (2.3) are both satisfied. \(\square\)

The next result gives another sufficient condition for $A$ to be cp.

**Theorem 2.2.** If

$$a_{ij} \geq a_{i4} a_{j4}, \quad 1 \leq i, j \leq 3,$$  

(2.7)

or

$$a_{ij} \geq a_{i5} a_{j5}, \quad 1 \leq i, j \leq 3,$$  

(2.8)

then $A$ is cp.
Proof. Suppose that (2.8) holds. We consider $S_5 := A/[a_{55}]$, the Schur complement of $[a_{55}]$ in $A$. Then

$$S_5 = [s_{ij}] = A(\{5\}) - \begin{bmatrix} a_2^T \\ 0 \end{bmatrix} [a_2^T, 0].$$

(2.9)

Therefore we have

$$s_{ij} = a_{ij} - a_{5i}a_{5j}, \quad 1 \leq i, j \leq 4,$$

(2.10)

where $a_{45} = a_{54} = 0$. From the hypothesis, we know that $s_{ij} \geq 0$ ($1 \leq i, j \leq 4$) and $S$ is also positive semidefinite (see, for example, [1]). Thus $S_5$ is dnn and hence cp, i.e., there exists some $4 \times 4$ nonnegative matrix $F$ such that $S_5 = FF^T$. By setting $B = \begin{bmatrix} F & a_2^T \\ 0 & 1 \end{bmatrix}$,

where $a_2^T = \begin{bmatrix} a_2^T \\ 0 \end{bmatrix}$, we get $A = BB^T$. Consequently we have $A \in CP_5$. The proof in the case that (2.7) holds is similar. □

Let $C$ be the Schur complement of $A_{22}$ in $A$, that is,

$$C = [c_{ij}] = A/A_{22} = A_{11} - A_{12}A_{12}^T.$$  

(2.11)

Since $A$ is psd, $C$ is also psd (e.g., [1, 5]). Nonnegativity is not inherited by Schur complements, so $C$ may have negative entries. Let $\mu = \mu(C)$ denote the number of negative entries above the diagonal of $C$. In the following section we will show that if $\mu \neq 2$, then $A$ is cp, and in Section 4 we study the case $\mu = 2$.

Proposition 2.3. Let $A = [a_{ij}] \in DNN_5$ be in form (2.1). Then

(a) There exists a nonnegative number $d$ such that $\tilde{A} := A - dE_{11}$ is dnn and singular.

(b) $A$ is cp if $\tilde{A}$ is cp.

(c) $A$ is singular if and only if $C = A/A_{22}$ is singular.

Proof. (a) If $A$ is singular, then we choose $d = 0$. If $A$ is nonsingular, then it is pd and so are all its principal submatrices. For

$$S = \begin{bmatrix} I_3 & 0 \\ -A_{12}^T A_{11}^{-1} & I_2 \end{bmatrix},$$

$$SAS^T = A_{11} \oplus (I_2 - A_{12}^T A_{11}^{-1} A_{12}).$$

Since $A \in PD_5$ implies $A_{11} \in PD_3$, it follows that

$$a_{11} > [a_{12}, a_{13}]A[2, 3]^{-1} \begin{bmatrix} a_{12} \\ a_{13} \end{bmatrix}.$$
Let
\[ d = a_{11} - [a_{12}, a_{13}]A[2, 3]^{-1} \begin{bmatrix} a_{12} \\ a_{13} \end{bmatrix}, \]
then \( d > 0 \) and \( \tilde{A} := A - dE_{11} \in \text{DNN}_4. \)

(b) \( A = \tilde{A} + \text{diag}(d, 0, 0, 0, 0). \)

(c) This follows from the formula \( \text{rank}(A) = \text{rank}(C) + 2 \) (Theorem 1.17 of [5]). \( \square \)

Proposition 2.3 will be used to deal with a subcase (Subcase 3) in the proof of Theorem 3.1, and before Theorem 4.2.

The following theorem gives a sufficient condition for a nonsingular matrix \( A \) in form (2.1) to be completely positive.

**Theorem 2.4.** Let \( A = [a_{ij}] \in \text{DNN}_5 \) be in form (2.1), where \( A_{11} \) is nonsingular.

Then \( A \) is cp if
\[ \alpha_1^T A_{11}^{-1} \alpha_1 + \alpha_2^T A_{11}^{-1} \alpha_2 \leq 1. \] \( (2.12) \)

**Proof.** Choose \( \lambda_1, \lambda_2 \in \mathbb{R} \) such that
1. \( \lambda_i \geq a_i^T A_{11}^{-1} a_i, i = 1, 2. \)
2. \( \lambda_1 + \lambda_2 = 1. \)

and denote \( B_i = \lambda_i A_{11} \) and
\[ A_i = \begin{bmatrix} a_{11} \\ a_i^T \\ \lambda_i \end{bmatrix}, \quad i = 1, 2. \] \( (2.13) \)

It is easy to see that \( B_i \in \text{DNN}_3, \) and \( A_i \in \text{DNN}_4 \) for \( i = 1, 2. \)
Furthermore, we have
\[ B_i - \alpha_i a_i^T = \lambda_i A_{11} - \alpha_i a_i^T = \lambda_i (A_{11} - \alpha_i \lambda_i^{-1} a_i^T) = \lambda_i (A_i/\lambda_i) \in \text{CP}_3, \]

where \( (A_i/\lambda_i) \) is the Schur complement of \( \lambda_i \) in \( A_i. \)
Therefore (2.2) and (2.3) are both satisfied by \( B_1, B_2. \) By Theorem 2.1, \( A \) is cp. \( \square \)

When \( C \) is not entrywise nonnegative, we define \( \lambda_4, \lambda_5 \) as
\[ \lambda_k = \min_{1 \leq i < j \leq 3} \left\{ a_{ik} a_{jk} c_{ij} : c_{ij} < 0 \right\}. \] \( (2.14) \)

It is obvious that \( \lambda_k \geq 0 \) for \( k = 4, 5. \)

We conclude the section by

**Theorem 2.5.** If \( C \) is not entrywise nonnegative and
\[ \lambda_4 + \lambda_5 \geq 1, \] \( (2.15) \)

then \( A \) is cp.
Proof. Denote
\[ C^{(1)} = \alpha_1 \alpha_1^T + \lambda_4 C = [c^{(1)}_{ij}], \quad C^{(2)} = \alpha_2 \alpha_2^T + \lambda_5 C = [c^{(2)}_{ij}]. \]
Then
\[ c^{(1)}_{ij} = a_{i4}a_{j4} + \lambda_4 c_{ij}, \quad c^{(2)}_{ij} = a_{i5}a_{j5} + \lambda_5 c_{ij}, \]
where \( i, j \in \{1, 2, 3\} \). By the definition of \( \lambda_4, \lambda_5 \), we have
\[ c^{(k)}_{ij} \geq 0, \quad i, j \in \{1, 2, 3\}, \quad k = 1, 2. \]
(2.17)
Being psd, \( C^{(k)} \) is dnn, and since it is a \( 3 \times 3 \) matrix, it is cp. By appropriate decreasing of \( \lambda_4, \lambda_5 \), we may assume \( \lambda_4 + \lambda_5 = 1 \), while keeping \( \lambda_4, \lambda_5 \geq 0 \) with (2.17) being satisfied. Consequently, we have
\[ A_{11} = C^{(1)} + C^{(2)}, \]
(2.18)
so by Theorem 2.1, \( A \) is cp. \( \square \)

3. The case \( \mu \neq 2 \)

In this section, we show

Theorem 3.1. If \( \mu \neq 2 \), then \( A \) is cp.

Proof. We consider the following three subcases according to the value of \( \mu \):

Subcase 1: \( \mu = 0 \). In this case \( C \) is entrywise nonnegative. Since \( A \) is psd, we know that \( C \) is also psd, and thus \( C \in \text{DNN}_3 \) because \( C \) is entrywise nonnegative. But \( \text{DNN}_3 = \text{CP}_3 \), so we have an entrywise nonnegative matrix of order 3, say \( D_1 \), such that \( C = D_1D_1^T \). By setting
\[ B_1 = \alpha_1 \alpha_1^T, \quad B_2 = [\alpha_2, D_1] \begin{bmatrix} \alpha_2^T \\ D_1 \end{bmatrix}, \]
we get (2.2). It is easy to check that (2.3) is also satisfied.

Subcase 2: \( \mu = 1 \). We may assume that the only negative entry above the main diagonal of \( C \) is \( c_{ij} \) where \( 1 \leq i < j \leq 3 \). Then by (2.14) we have
\[ \lambda_4 + \lambda_5 = \frac{a_{i4}a_{j4} + a_{i5}a_{j5}}{a_{i4}a_{j4} + a_{i5}a_{j5} - a_{ij}} \geq 1. \]
(2.17)
It follows from Theorem 2.5 that \( A \) is cp.

Subcase 3: \( \mu = 3 \). In this case \( C \) is a Z-matrix, and therefore it is an M-matrix (since it is also psd). We may assume that \( C \) is singular since otherwise we may decrease the first diagonal entry of \( A_{11} \) to make \( A \), and consequently \( C \), singular, without changing the complete positivity of \( A \) (e.g., Proposition 2.3) and the off-diagonal
entries of $C$. Therefore we may find some positive vector $v = (v_1, v_2, v_3)^T \in \mathbb{R}_+^3$ such that $Cv = 0$. Denote

$$b_{ij}^{(1)} = \frac{a_{ij}a_4a_5}{a_4a_4 + a_5a_5}, \quad b_{ij}^{(2)} = \frac{a_{ij}a_5a_j}{a_4a_4 + a_5a_5}, \quad i \neq j,$$

and for $i = j \in \{1, 2, 3\}$, we define

$$b_{ii}^{(1)} = a_{i4}^2 + \sum_{j=1, j \neq i}^3 \frac{v_j}{v_i} (a_4a_j - b_{ij}^{(1)})$$

and

$$b_{ii}^{(2)} = a_{i5}^2 + \sum_{j=1, j \neq i}^3 \frac{v_j}{v_i} (a_5a_j - b_{ij}^{(2)}).$$

Simple calculation shows that $B_1 = [b_{ij}^{(1)}], B_2 = [b_{ij}^{(2)}]$ are both dnn, and also $B_i - \alpha_i \alpha_i^T \in \text{PSD}_3$ for $i = 1, 2$. It is not difficult to check that both (2.2) and (2.3) are satisfied, and this completes the proof. \(\Box\)

It is worth mentioning that $\text{cp-rank}(A) \leq 5$ when $\mu = 0$. As a matter of fact, if we set $\beta_1 = [\alpha_1^T, 1, 0]^T$ and $A_1 = \beta_1 \beta_1^T$, we have

$$A_2 = A - A_1 = \begin{bmatrix} B_2 & 0 & \alpha_2 \\ 0 & 0 & 0 \\ \alpha_2^T & 0 & 1 \end{bmatrix} \in \text{CP}_3.$$ 

Since $\text{cp-rank}(A_2) \leq 4$ (see, for example, [7]), we have $\text{cp-rank}(A) \leq 5$. Moreover, $\text{cp-rank}(A) = 5$ when $C$ is pd (or equivalently, $A$ is pd).

4. The case $\mu = 2$

Since $\mu = 2$, we may always assume in the following, by some suitable permutation, that

$$c_{12} > 0, \quad c_{13} < 0, \quad c_{23} < 0.$$

**Proposition 4.1.** Let $\mu = 2$. If

$$\lambda_4 + \lambda_5 < 1,$$

then either

$$\frac{a_{14}}{a_{24}} < \frac{c_{13}}{c_{23}} < \frac{a_{15}}{a_{25}}$$

or

$$\frac{a_{15}}{a_{25}} < \frac{c_{13}}{c_{23}} < \frac{a_{14}}{a_{24}}.$$
Proof. Suppose (4.1) holds. Suppose also that
\[ \lambda_4 = \frac{a_{14}a_{34}}{-c_{13}}, \]  
(4.4)
or equivalently,
\[ \frac{a_{14}a_{34}}{-c_{13}} \leq \frac{a_{24}a_{34}}{-c_{23}}. \]  
(4.5)
If \( a_{34} = 0 \), then \( \lambda_4 = 0 \). It follows from the definition of \( \lambda_5 \) that
\[ \lambda_5 = \frac{a_{5a_j}}{a_{5a_j} - a_{ij}} \geq 1 \]
for some \( 1 \leq i < j \leq 3 \), a contradiction to (4.1). If the equality in (4.5) holds, then we have
\[ \lambda_4 = \frac{a_{14}a_{34}}{-c_{13}} = \frac{a_{24}a_{34}}{-c_{23}}, \]
which implies (2.15), contradicting (4.1). Therefore, we may rewrite (4.5) as
\[ \frac{a_{14}}{a_{24}} < \frac{c_{13}}{c_{23}}. \]  
(4.6)
We can also apply a similar argument to \( \lambda_5 \) while keeping (4.1) in mind to get
\[ \frac{c_{13}}{c_{23}} < \frac{a_{15}}{a_{25}}. \]  
(4.7)
Thus (4.2) is proved. In the case
\[ \lambda_4 = \frac{a_{24}a_{34}}{-c_{23}}, \]  
(4.8)
we can prove (4.3) in a similar way. □

Note that the converse of Proposition 4.1 is not necessarily true, as the following example shows.

Example 4.1. Let
\[
A = \begin{bmatrix}
6 & 5 & 5 & 1 & 2 \\
5 & 6 & 5 & 2 & 1 \\
5 & 5 & 9 & 2 & 2 \\
1 & 2 & 2 & 1 & 0 \\
2 & 1 & 2 & 0 & 1
\end{bmatrix}.
\]
An easy computation yields
\[
C = \begin{bmatrix}
1 & 1 & -1 \\
1 & 1 & -1 \\
-1 & -1 & 1
\end{bmatrix}; \quad \lambda_4 = \lambda_5 = 2,
\]
but (4.2) holds.
Now suppose $A$ is singular. By Proposition 2.3, $C$ is also singular. Since $\mu = 2$ implies $C \neq 0$, $\text{rank}(C) = 1$ or $2$. The following theorem settles the case $\text{rank}(C) = 1$.

**Theorem 4.2.** Suppose $\mu(C) = 2$ and $\text{rank}(C) = 1$. Then $A \in \text{CP}_5$ if and only if (2.15) holds.

**Proof.** Suppose (2.15) holds. Since $\lambda_4, \lambda_5 \geq 0$, there exists some real number $\lambda$ such that $0 \leq \lambda \leq 1$ and $1 - \lambda_5 \leq \lambda \leq \lambda_4$. By the definition of $\lambda_k$, we get

$$
\begin{pmatrix}
a_{14}a_{34} - a_{13} \\
a_{24}a_{34} - a_{23}
\end{pmatrix} \leq \lambda \begin{pmatrix}
-c_{13} \\
-c_{23}
\end{pmatrix} \leq \begin{pmatrix}
a_{14}a_{34} \\
a_{24}a_{34}
\end{pmatrix},
$$

(4.9)

which implies

$$
a_{34} \begin{pmatrix} a_{14} \\ a_{24} \end{pmatrix} + \lambda \begin{pmatrix} c_{13} \\ c_{23} \end{pmatrix} \geq 0
$$

(4.10)

and

$$
a_{35} \begin{pmatrix} a_{15} \\ a_{25} \end{pmatrix} + (1 - \lambda) \begin{pmatrix} c_{13} \\ c_{23} \end{pmatrix} \geq 0.
$$

(4.11)

Denote

$$
B_1 = \alpha_1 \alpha_1^T + \lambda C, \quad B_2 = \alpha_2 \alpha_2^T + (1 - \lambda)C.
$$

(4.12)

It follows from (4.11) and (4.12) that $B_1, B_2$ are dnn. Furthermore, we have (2.2) and (2.3). Consequently, $A \in \text{CP}_5$ by Theorem 2.1.

We now prove the necessity. Suppose $A \in \text{CP}_5$, then by Theorem 2.1, there exist $B_1, B_2 \in \text{DNN}_3$ such that both (2.2) and (2.3) are satisfied. Denote

$$
C_i = B_i - \alpha_i \alpha_i^T, \quad i = 1, 2.
$$

Then by (2.3) $C_i$ is psd for $i = 1, 2$. It is easy to check that

$$
C = C_1 + C_2.
$$

(4.13)

We want to prove the following assertion:

---

**C has a decomposition (4.13) with $C_1, C_2$ being psd if and only if there exists some real number $\lambda : 0 \leq \lambda \leq 1$ such that $C_1 = \lambda C, C_2 = (1 - \lambda)C$.**

---

In fact, since $\text{rank}(C) = 1$ and $C, C_1, C_2$ are all psd, we know that the assertion is true because any psd matrix of rank 1 is obviously an extreme vector of the cone $PSD_3$. If we denote $B_i = C_i + \alpha_i \alpha_i^T, i = 1, 2$, then $B_1, B_2 \in \text{DNN}_3$. From the proof of the sufficiency, we get (4.10) and (4.11) (since $B_1, B_2$ are entrywise nonnegative), which is followed by (4.9). But (4.9) is identical to (2.15). The proof is completed. \( \square \)

Before we state the following result, let us define some notations. Let $M$ be an $n \times n$ matrix. Let $1 \leq i_1 < i_2 \leq n, 1 \leq j_1 < j_2 \leq n$. We shall denote by $M[i_1, i_2, j_1, j_2]$
the submatrix of $M$ lying in rows $i_1, i_2$ and columns $j_1, j_2$, and $M[i_1, i_2]$ the submatrix $M[i_1, i_2][j_1, j_2]$. For convenience, we define $\det M[i_1, i_2]$ to be 0.

The following theorem gives a sufficient condition for $A$ to be cp, where $\text{rank}(C) = \mu(C) = 2$. For simplicity, we assume in the theorem, without loss of generality, that $c_{12} > 0$ (otherwise, we may use some appropriate similarity permutation).

**Theorem 4.3.** Let $\text{rank}(C) = \mu(C) = 2$, and suppose that the only positive element above the main diagonal of $C$ is $c_{12}$, Then $A \in \text{CP}_3$ if

$$\det C[1, 2|1, 3] \geq 0.$$  \hspace{1cm} (4.14)

**Proof.** Denote the adjoint matrix of $C$ by $\text{adj} C$. Then we have

$$\text{rank(\text{adj} C)} = 1$$ \hspace{1cm} (4.15)

since $\text{rank}(C) = 2$. Hence any 2 by 2 submatrix of $\text{adj} C$ is singular. Also we have $c_{ii} > 0$ for all $i \in \{1, 2, 3\}$ since otherwise $\mu(C) \neq 2$. Furthermore, $\text{adj} C$ is psd (in fact, $\text{adj} C = vv^T$ for some nonzero vector $v \in \mathbb{R}^3$). Denote

$$\beta_1 = \begin{bmatrix} \sqrt{\text{det} C[1, 1]} / c_{11}, & \sqrt{\text{det} C[1, 2]} / c_{11}, & \sqrt{\text{det} C[1, 3]} / c_{11} \end{bmatrix}^T,$$

$$\beta_2 = \begin{bmatrix} c_{11} / \sqrt{c_{11}}, & c_{12} / \sqrt{c_{11}}, & c_{13} / \sqrt{c_{11}} \end{bmatrix}^T$$ \hspace{1cm} (4.16)

and let $B_k = \alpha_k \alpha_k^T + \beta_k \beta_k^T, k = 1, 2$. Observe that the first entry of $\beta_1$ is 0. It is not difficult to see that $B_1$ is dnn while $B_2$ is psd (but is not necessarily dnn since $\mu(C) = 2$ implies $c_{13} < 0, c_{23} < 0$).

In fact, if $B_2$ is dnn, i.e., it is also nonnegative, then

$$\lambda_{13}^{(2)} = a_{13} - a_{14}a_{34} \geq 0,$$

which is followed by $a_{13} \geq a_{14}a_{34}$, and

$$0 \leq b_{23}^{(2)} = a_{25}a_{35} + c_{12}c_{13}/c_{11} \leq a_{25}a_{35} + c_{23} = a_{23} - a_{24}a_{34},$$

[note that $c_{12}c_{13}/c_{11} = c_{23} - \det C[1, 2|1, 3]/c_{11} \leq c_{23}$ due to (4.14)] which follows from $a_{23} \geq a_{24}a_{34}$. Consequently we get (2.7) (since $c_{12} > 0$ implies $a_{12} \geq a_{14}a_{24}$, and thus $A$ is cp by Theorem 2.2.

So we need only to consider the case when $B_2$ is not nonnegative. From the above discussion, this is equivalent to say that either

$$a_{13} < a_{14}a_{34}$$ \hspace{1cm} (4.18)

or

$$a_{23} < a_{24}a_{34} + \frac{\det C[1, 2|1, 3]}{c_{11}}.$$ \hspace{1cm} (4.19)
We observe that

\[ B_1 + B_2 = \alpha_1 \alpha_1^T + \alpha_2 \alpha_2^T + \beta_1 \beta_1^T + \beta_2 \beta_2^T = \tilde{C} + A_{12} A_{21}, \]

where

\[ \tilde{C} = \beta_1 \beta_1^T + \beta_2 \beta_2^T = [\tilde{c}_{ij}], \]

with \( C_1 = [\beta_1, \beta_2]^T \in \mathbb{R}^{2 \times 3} \) (note that \( C_1 \) is not necessarily entrywise nonnegative).

We want to prove that \( \tilde{C} = C \) so that (2.2) is satisfied. As a matter of fact, we have \( \tilde{c}_{1j} = \tilde{c}_{j1} = c_{1j} = c_{j1} \) for all \( j = 1, 2, 3 \). For any \( i \neq 1, j \neq 1 \), we have

\[ \tilde{c}_{ij} = \frac{1}{c_{11}} (c_{1i} c_{1j} + \sqrt{\det C[1,i] \det C[1,j]}). \]  

By (4.16) we get

\[ 0 = \det \adj C[1,i][1,j] = \det C[1,i] \det C[1,j] - (\det C[1,i][1,j])^2. \]

This implies \( (c_{11} c_{1j} - c_{1i} c_{1j})^2 = \det C[1,i] \det C[1,j] \). Thus we have \( \tilde{c}_{ij} = c_{ij} \) for any \( i, j \in \{1, 2, 3\} \). Therefore (2.2) is satisfied. Now we denote

\[ \beta'_1 = \beta_1 \cos \theta + \beta_2 \sin \theta, \quad \beta'_2 = \beta_2 \cos \theta - \beta_1 \sin \theta, \]

and

\[ B^{(k)} = [b_{ij}^{(k)}] = \beta'_1 \beta'_2^T + \alpha_k \alpha_k^T, \quad k = 1, 2. \]

Then it is easy to check that

\[ A_{11} = C + A_{12} A_{21} = B^{(1)} + B^{(2)}. \]

It suffices to find a \( \theta \) \((-\frac{\pi}{2} < \theta < \frac{\pi}{2})\) such that both \( B^{(1)} \) and \( B^{(2)} \) are nonnegative, i.e., \( 0 \leq B^{(1)} \leq A_{11} \) \((X \leq Y \) implies \( x_{ij} \leq y_{ij} \) for all \( i, j \) when the two matrices \( X, Y \) are of the same order). This can be rewritten in detail as

\[ -a_{i4} a_{j4} \leq \frac{1}{c_{11}} (c_{1i} \sin \theta + \sqrt{\det C[1,i] \cos \theta}) (c_{1j} \sin \theta + \sqrt{\det C[1,j] \cos \theta}) \leq a_{ij} - a_{i4} a_{j4} \]

for \( 1 \leq i < j \leq 3 \). Now we denote \( t = \tan \theta \) and

\[ \lambda_k = \frac{\sqrt{\det C[1,k]}}{c_{11}^{\lambda_k}}, \]

for \( k = 1, 2, 3 \) (note that \( \lambda_1 = 0, \lambda_2 > 0, \lambda_3 < 0 \)). We can rewrite (4.24) as

\[ -a_{14} a_{24} \leq \frac{c_{12} t (\lambda_2 + \lambda_3)}{t^2 + 1} \leq a_{12} - a_{14} a_{24}, \]

\[ -a_{14} a_{34} \leq \frac{c_{13} t (\lambda_2 + \lambda_3)}{t^2 + 1} \leq a_{13} - a_{14} a_{34}, \]

\[ -a_{24} a_{24} \leq \frac{c_{12} c_{13} (t + \lambda_2)(t + \lambda_3)}{c_{11} t^2 + 1} \leq a_{23} - a_{24} a_{34}. \]
By some elementary (however tedious) calculations, while keeping the hypotheses (4.14), (4.19) and (4.20) in mind, we know that there exists some θ in $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$ such that (4.25)–(4.27) hold. The proof is completed by choosing such a θ so that (2.2) and (2.3) are satisfied by $B^{(1)}, B^{(2)}$. □

Theorem 4.3 states that (4.14) is a sufficient condition. The question whether it is also necessary is still open. We think that it is and state it as a conjecture at the end of the paper.

5. The reduction of $A$ to the cases with more than 2 zeros

In this section, we will deal with the case when $\mu(C) = \text{rank}(C) = 2$ and neither (2.7) nor (2.8) holds. In this case, there exist two pairs of indices, $(i_1, j_1), (i_2, j_2)$ such that $1 \leq i_t < j_t \leq 3, t = 1, 2$ and

$$a_{i_t,j_t} < a_{i_t,3+i} a_{i_t,3+i}, \quad t = 1, 2. \quad (5.1)$$

We consider two subcases:

Subcase 1: $(i_1, j_1) = (i_2, j_2)$. Since $e_{12} > 0$, we may assume that $(i_1, j_1) = (1, 3), (i_2, j_2) = (2, 3)$. In this case, (5.1) is equivalent to

$$a_{i,3} < a_{i,3+i} a_{3,3+i}, \quad i = 1, 2. \quad (5.2)$$

Write $\mu_{i,3} = \frac{a_{i,3} - a_{i,3+i}}{a_{i,3+i}}$ and $S_{i,3} = I_5 - \mu_{i,3} E_{i,3+i}, i = 1, 2$. Simple calculation yields

$$\hat{A} := (S_{23} S_{13}) A (S_{23} S_{13})^T = \begin{bmatrix}
a'_{i,1} & a'_{12} & 0 & a'_{4} & a'_{5} \\
a'_{21} & a'_{22} & 0 & a_{24} & a'_{25} \\
0 & 0 & 1 & a_{34} & a_{35} \\
a'_{41} & a_{42} & a_{43} & 1 & 0 \\
\mu_{i,3} & a'_{51} & a'_{52} & a_{53} & 0 & 1
\end{bmatrix}, \quad (5.3)$$

where

$$a'_{i,i} = 1 + \mu_{i,3}^2 - 2a_{i,3+i} \mu_{i,3}, \quad i = 1, 2, \quad (5.4)$$

and

$$a'_{12} = a'_{21} = a_{12} - \frac{a_{13} a_{24}}{a_{34}}, \quad (5.5)$$

$$a'_{i,3+i} = a'_{3+i,i} = a_{i,3+i} - \frac{a_{i,3}}{a_{3,3+i}}, \quad i = 1, 2. \quad (5.6)$$

It follows from (5.2)–(5.6) that $\hat{A} \in \text{DNN}_5$. The graph $G(\hat{A})$ is an example of a book graph (e.g., [2,5]). For a book graph $G$ it is known how to determine if a dnn $n \times n$ matrix $A$, with $G(A) = G$, is cp or not. If $\hat{A}$ is cp, then $A$ is also cp.
Subcase 2: \((i_1, j_1) \equiv (i_2, j_2)\), and there exists no other pair of indices such that (5.1) holds. Since \(c_{12} > 0\), we may assume that \((i_1, j_1) = (i_2, j_2) = (1, 3)\), i.e.,
\[
\frac{a_{13}}{a_{1, (3+j)}} < \frac{a_{23}}{a_{2, (3+j)}} , \quad j = 1, 2.
\]
(5.7)
By setting \(S_{24} = I_5 - a_{24}E_{24}\), we readily get
\[
\tilde{A} := S_{24}AS_{24}^T = \begin{bmatrix}
1 & a'_{12} & a_{13} & a_{14} & a_{15} \\
a'_{21} & a'_{22} & a'_{23} & 0 & a_{25} \\
a_{31} & a'_{32} & 1 & a_{34} & a_{35} \\
a_{41} & 0 & a_{43} & 1 & 0 \\
a_{51} & a_{52} & a_{53} & 0 & 1
\end{bmatrix},
\]
(5.8)
where
\[
a'_{22} = 1 - a_{24}^2, \quad (5.9)
\]
\[
a'_{12} = a'_{21} = a_{12} - a_{14}a_{24}, \quad (5.10)
\]
\[
a'_{23} = a'_{32} = a_{23} - a_{24}a_{34}. \quad (5.11)
\]
It follows from (5.7)–(5.11) that \(\tilde{A} \in \text{DNN}_5\). The graph \(G(\tilde{A})\) is also a book graph, and here too, \(A\) is cp if \(\tilde{A}\) is cp.

It is not clear yet how to determine if \(A\) is completely positive when \(\tilde{A}\) (or \(\tilde{A}\)) is not cp.

6. Positive dnn matrices

A matrix \(\tilde{A}\) is called an edge-deleted matrix of \(A \in \text{DNN}_n\) if there exists some positive number \(\nu\) and some index pair \((i, j)\) with \(i \neq j, 1 \leq i, j \leq n\) such that \(\tilde{A} := SAS^T \in \text{DNN}_n\), and \(G(\tilde{A})\) is a subgraph of \(G(A)\) obtained by deleting at least one of its edges \((V[G(\tilde{A})] = V[G(A)])\), where \(S = I_n - \nu E_{ij}\) (see [9]).

We first show that a positive matrix \(A \in \text{DNN}_5\) is cp if and only if there exists an edge-deleted matrix of \(A\), which is cp.

**Theorem 6.1.** Let \(A = [a_{ij}] \in \text{DNN}_5\), and \(G(A) = K_5\) (i.e., \(a_{ij} > 0\) for all \(i, j\)). Then \(A\) is cp if and only if there exists an edge-deleted matrix of \(A\), \(\tilde{A}\), which is cp.

**Proof.** “Sufficiency” Since \(\tilde{A} \in \text{CP}_5\), we have \(\tilde{A} = BB^T\) for some \(S \times m\) \((m = \text{cp-rank}(A))\) entrywise nonnegative matrix \(B\), and thus
\[
A = S^{-1}\tilde{A}(S^{-1})^T = (S^{-1}B)(S^{-1}B)^T.
\]
Note that since \(S^{-1}\) is entrywise nonnegative, we know that \(A\) is cp.

“Necessity” Suppose \(A = [a_{ij}] \in \text{CP}_5\) with \(G(A) = K_5\). We may assume that \(a_{ii} = 1\) for all \(i = 1, \ldots, 5\). Then we have some unit vectors \(\alpha_1, \ldots, \alpha_5 \in R^m_+\) (where \(m = \text{cp-rank}(A)\)) such that \(A = \text{Gram}(\alpha_1, \ldots, \alpha_5)\), that is,
\[
(a_i, a_j) = a_{ij}, \quad 1 \leq i, j \leq 5. \tag{6.1}
\]
If there is some \(a_{ij} = 1\) for some \(i \neq j\), we may assume that \(i < j\). Then we have \(a_i = a_j\). In fact, the equality in
\[
(a_i, a_j)^2 \leq (a_i, a_i)(a_j, a_j) \tag{6.2}
\]
holds if and only if \(a_i = c a_j\) for some real number \(c\). Furthermore, we have \(c = 1\) from \(\|a_i\| = \|a_j\| = 1\). Therefore, \(a_i = a_j\). By setting \(S = I_5 - E_{ij}, \tilde{A} = SAS^T\), we easily get \(G(\tilde{A}) = K_4 \cup \{i\}\), showing that \(\tilde{A}\) is truly an edge-deleted matrix of \(A\). On the other hand, \(\tilde{A}\) is permutation similar to the matrix \(0 \oplus A(i|j)\), which is obviously cp. Thus we need only to consider the case \(0 < a_{ij} < 1\) for all \(i, j = 1, \ldots, 5, i \neq j\). The following discussion is based on this assumption.

We now define
\[
\theta_{ij} = \arccos a_{ij}, \quad 1 \leq i, j \leq 5. \tag{6.3}
\]
Then we have \(0 < \theta_{ij} < \pi/2\) for all \(i, j = 1, \ldots, 5, i \neq j\). Next we denote
\[
\theta = \max \{\theta_{ij}, i, j = 1, \ldots, 5\}. \tag{6.4}
\]
Obviously \(0 < \theta < \pi/2\). We may suppose, without loss of generality, that \(\theta = \theta_{12}\). We may use a unitary rotation, if necessary, such that \(\alpha_2\) lies in a coordinate hyperplane. Now we fix \(\alpha_2, \alpha_3, \alpha_4, \alpha_5\) and rotate \(\alpha_1\) to the position \(\alpha'_1\) such that

(1) \(\alpha'_1, \alpha_1, \alpha_2\) are in the same hyperplane, denoted by \(H\),
(2) \(\alpha'_1\) is perpendicular to the vector \(\alpha_2\).

Now we let \(\tilde{A} = \text{Gram}(\alpha'_1, \alpha_2, \ldots, \alpha_5)\). Then \(\tilde{A}\) is cp. It suffices to prove the matrix \(\tilde{A}\) is an edge-deleted matrix of \(A\), i.e., there exists some positive number \(\delta\) and a pair of indices \((i, j)\) with \(i \neq j, 1 \leq i, j \leq 5\) such that \(\tilde{A} := SAS^T\) where \(\tilde{S} = I_5 - \delta E_{ij}\). By denoting
\[
v = \min \left\{ \frac{a_{ij}}{a_{2j}} : 1 \leq j \leq 5 \right\}, \tag{6.5}
\]
we have \(v = a_{12}\) since otherwise we have \(v = \frac{a_{it}}{a_{2t}}\) for some \(t \in \{3, 4, 5\}\), and \(a_{12} > \frac{a_{1t}}{a_{2t}} > a_{1i}\), contradicting the hypothesis. Therefore we have \(v = a_{12}\). By setting \(S = I_5 - v E_{12}, \tilde{A} = SAS^T = [\tilde{a}_{ij}]\), we need only to prove that \(\tilde{A} = \tilde{A}\), that is,
\[
\tilde{a}_{ij} = (\alpha'_i, \alpha'_j), \quad i, j = 1, \ldots, 5.
\]
For \(2 \leq i, j \leq 5\), it is obvious that
\[
\tilde{a}_{ij} = a_{ij} = (a_i, a_j) = (\alpha'_i, \alpha'_j).
\]
For \(i = 1\), since \(\alpha'_1, \alpha_2\) are orthogonal, and \(\alpha_1\) lies in the hyperplane, the angle between \(\alpha_1\) and \(\alpha_2\) is \(\theta_{12} = \theta\). Simple geometric observation yields
\[
\alpha_1 = \alpha'_1 \sin \theta_{12} + \alpha_2 \cos \theta_{12}, \tag{6.6}
\]
which can be equivalently expressed as
\[ \alpha_1' = \frac{\alpha_1 - \alpha_2 \cos \theta_{12}}{\sin \theta_{12}}. \] (6.7)

Thus we have
\[
(a_1', a_j') = (a_1', a_j) = \frac{a_{1j} - a_{12}a_{2j}}{\sqrt{1 - a_{12}^2}} = \frac{a_{1j} - \nu a_{2j}}{\sqrt{1 - 2a_{12}^2 + \nu^2}} = \tilde{a}_{1j}.
\]

Therefore we have \( \tilde{A} = \hat{A} \), and the proof is completed. \( \square \)

7. Summary

Let \( A = [a_{ij}] \) be any dnn \( 5 \times 5 \) matrix. If \( A \) is positive, then we can replace \( A \) by \( \hat{A} \), defined in the proof of Theorem 6.1. Then \( A \) is cp if and only if \( \tilde{A} \) is cp. If \( A \) is dnn but not positive, we can put it in form (2.1), using permutation similarity and nonnegative diagonal scaling, if necessary. So it suffices to consider the case when \( A \) is a dnn matrix in form (2.1). We have the following sufficient conditions for \( A \) to be cp in this case:

1. If (2.7) holds, then \( A \) is cp (Theorem 2.2).
2. If (2.8) holds, then \( A \) is cp (Theorem 2.2).
3. If neither (2.7) nor (2.8) holds, and \( \hat{A} \) defined in Section 5 is cp, then \( A \) is cp.
4. If neither (2.7) nor (2.8) holds, and \( \tilde{A} \) defined in Section 5 is cp, then \( A \) is cp.
5. If \( A_{11} \) is nonsingular, and (2.12) holds, then \( A \) is cp (Theorem 2.4).
6. If \( \mu(C) \neq 2 \), where \( C \) is given by (2.11) and \( \mu = \mu(C) \) is the number of negative entries above the diagonal of \( C \), then \( A \) is cp (Theorem 3.1).
7. If \( \mu(C) = 2 \), \( \text{rank}(C) = 2 \) and (4.14) holds, then \( A \) is cp (Theorem 4.3).
8. If \( \mu(C) = 2 \), \( \text{rank}(C) = 1 \) and \( \lambda_4 + \lambda_5 \geq 1 \), where \( \lambda_4 \) and \( \lambda_5 \) are defined by (2.14), then \( A \) is cp (in fact, in this case, \( \lambda_4 + \lambda_5 \geq 1 \) is also necessary) (Theorem 4.2).

Open Problems. The characterization of CP5 will be completed if the following two conjectures could be proved:

- **Conjecture 1:** If \( A \in \text{DNN}_5 \) satisfies \( \mu(C) = \text{rank}(C) = 2 \), then \( A \) is cp if and only if (4.14) holds (the 'only if' part remains open).
Conjecture 2: A nonsingular dnn matrix $A$ in form (2.1) can always be reduced, by decreasing some of the diagonal entries of $A_{11}$, to a singular dnn matrix $\tilde{A}$, such that $A$ is cp if and only if $\tilde{A}$ is cp (the ‘if’ part is true by Proposition 2.3).

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References