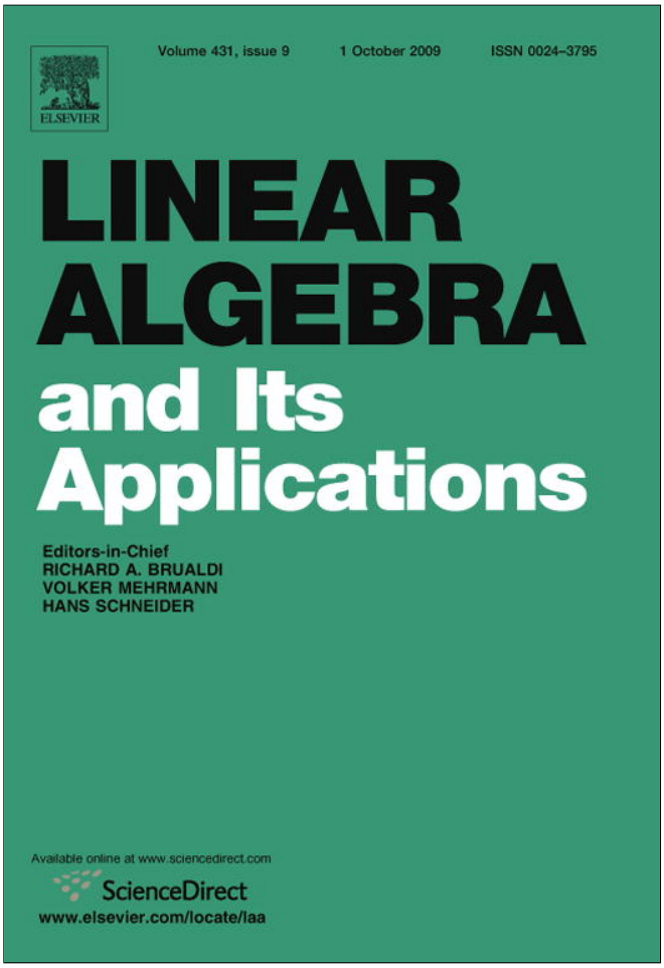
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The difference between 5 × 5 doubly nonnegative and completely positive matrices

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A B S T R A C T

The convex cone of $n \times n$ completely positive (CP) matrices and its dual cone of copositive matrices arise in several areas of applied mathematics, including optimization. Every CP matrix is doubly nonnegative (DNN), i.e., positive semidefinite and component-wise nonnegative, and it is known that, for $n \leqslant 4$ only, every DNN matrix is CP. In this paper, we investigate the difference between 5×5 DNN and CP matrices. Defining a *bad* matrix to be one which is DNN but not CP, we: (i) design a finite procedure to decompose any $n \times n$ DNN matrix into the sum of a CP matrix and a bad matrix, which itself cannot be further decomposed; (ii) show that every bad 5×5 DNN matrix is the sum of a CP matrix and a single bad extreme matrix; and (iii) demonstrate how to separate bad extreme matrices from the cone of 5×5 CP matrices.

1. Introduction

The convex cone of completely positive matrices has long been of interest in several fields of mathematics [2]. Recently, it has attracted interest in optimization where it has been shown that NP-hard nonconvex quadratic programs, possibly also containing binary variables, may be reformulated as linear optimization problems over this cone [5].

Let $\mathcal{S}_n$ denote the set of $n \times n$ symmetric matrices, and $\mathcal{S}_n^+$ denote the set of $n \times n$ symmetric, positive semidefinite matrices. We write $X \geqslant 0$ to mean that a matrix X is entrywise nonnegative and

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$X \succeq 0$ to mean $X \in \mathcal{S}_n^+$. An $n \times n$ matrix X is called completely positive (CP) if it can be decomposed as $X = NN^T$ for some $N \geqslant 0$. Clearly, each CP matrix is nonnegative and positive semidefinite, i.e., doubly nonnegative (DNN), but the reverse is not necessarily the case. Indeed, defining the closed convex cones

$$\mathcal{C}_n := \{X \in \mathcal{S}_n : X = NN^T \text{ for some } N \geqslant 0\},$$
$$\mathcal{D}_n := \{X \in \mathcal{S}_n : X \succeq 0, X \geqslant 0\},$$

of $n \times n$ CP and DNN matrices, respectively, it is known (cf. [11]) that for $n \leqslant 4$ only, $\mathcal{C}_n = \mathcal{D}_n$. The 5×5 case is therefore of particular interest and has received special attention [3,10,12]. Xu [12] has proposed criteria for a 5×5 DNN matrix to be CP based on the structure of an associated graph, whereas Berman and Xu [3] have given conditions based on the Schur complement.

In this paper, we assume throughout that $n \geqslant 5$. Our goal is to understand the nonempty set $\mathcal{D}_n \setminus \mathcal{C}_n$, in particular for the case $n = 5$. We will call any matrix in $\mathcal{D}_n \setminus \mathcal{C}_n$ a *bad* matrix. This terminology reinforces the perspective from optimization applications involving CP matrices [5], where $\mathcal{C}_n$ is the true domain of interest and $\mathcal{D}_n$ serves only as a (tractable) approximation of $\mathcal{C}_n$. In a sense, our work is related to that of Johnson and Reams [9] who study the dual cones $\mathcal{D}_n^*$ and $\mathcal{C}_n^*$ of $\mathcal{D}_n$ and $\mathcal{C}_n$. The cone $\mathcal{D}_n^*$ is the collection of all symmetric matrices that can be written as the sum of a component-wise nonnegative symmetric matrix and a positive semidefinite matrix, while $\mathcal{C}_n^*$ is the cone of copositive matrices, i.e., the set of all matrices A for which $x \geqslant 0$ implies $x^TAx \geqslant 0$. Johnson and Reams study $\mathcal{C}_n^* \setminus \mathcal{D}_n^*$. They call matrices in this set *exceptional matrices* and investigate methods to construct such matrices.

In Section 2 we consider the extreme rays of $\mathcal{D}_5$. We describe a new factorization that exists for any extreme $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$, which we term an *extremely bad* matrix. In Section 3 we consider the problem of "reducing" a matrix $X \in \mathcal{D}_n$ by decomposing X into the form $X = Y + Z$, where $0 \neq Y \in \mathcal{C}_n$ and $Z \in \mathcal{D}_n$. If such a decomposition exists we say that X is *CP-reducible*. We give a checkable characterization of CP-reducibility and use this characterization to devise a finite algorithm for CP-reduction. The output of the algorithm, with input $X \in \mathcal{D}_n$, is a decomposition $X = Y + Z$, where $Y \in \mathcal{C}_n, Z \in \mathcal{D}_n$, and Z is CP-irreducible. In Section 4 we prove that $X \in \mathcal{D}_5$ is CP-irreducible if and only if X is extremely bad. It follows that any $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ can be written in the form $X = Y + Z$, where $Y \in \mathcal{C}_5$ and Z is extremely bad, and such a decomposition can be found using the CP-reduction algorithm of Section 3. Finally, in Section 5 we show how to construct a linear hyperplane (or "cut") that separates a given extremely bad matrix from the cone of CP matrices. We give an example to show the positive effect that adding this cut can have when the solution of a relaxed optimization problem posed over $\mathcal{D}_5$ is not in $\mathcal{C}_5$.

We use the following terminology and notation. For a convex cone $\mathcal{K}$, $\text{Ext}(\mathcal{K})$ denotes the set of extreme rays of $\mathcal{K}$. It is well known that $\text{Ext}(\mathcal{C}_n) = \{vv^T : v \in \mathbb{R}_+^n\}$. The cone generated by a set of points $\mathcal{T}$ is denoted $\text{Cone}(\mathcal{T})$. For an $m \times n$ matrix X we use X_{IJ} to denote the submatrix of X corresponding to rows $i \in I$ and columns $j \in J$, where $I \subset \{1, \ldots, m\}$ and $J \subset \{1, \ldots, n\}$. We use $X_{I\cdot}$ and $X_{\cdot J}$ to denote the submatrices of X formed using the rows from I and columns from J, respectively. The range, nullspace and rank of a matrix X are denoted $\text{Range}(X)$, $\text{Null}(X)$ and $\text{rank}(X)$, respectively. For a vector $v \in \mathbb{R}^n$, $\text{Diag}(v)$ is the $n \times n$ diagonal matrix whose iith entry is v_i. The all-ones vector (of appropriate dimension) is denoted by e. For matrices A and B of the same size, $A \circ B$ denotes the Hadamard (componentwise) product and $A \bullet B$ denotes the matrix inner product, $A \bullet B = e^T(A \circ B)e$. For $X \in \mathcal{S}_n$, $G(X)$ is the simple graph on the vertices $\{1, \ldots, n\}$ associated with the nonzero entries of X, i.e., $G(X) = (\{1, \ldots, n\}, E)$, where $E = \{\{i,j\} : i \neq j, X_{ij} \neq 0\}$. We call a matrix $X \in \mathcal{S}_n$ cyclic if $G(X)$ is a cycle of length n.

2. The extreme rays of $\mathcal{D}_5$

In this section, we consider the extreme rays of $\mathcal{D}_5$. We begin with results from the literature that characterize $X \in \text{Ext}(\mathcal{D}_5)$ in terms of $\text{rank}(X)$ and $G(X)$. The first result establishes the existence of extreme matrices in $\mathcal{D}_n$ of nearly every rank, with rank 2 and ranks near n being the only exceptions.

Theorem 1. [8, Theorem 3.1] *Let $k \geqslant 1$. The set $\{X \in \text{Ext}(\mathcal{D}_n) : \text{rank}(X) = k\}$ is nonempty if and only if $k \neq 2$ and*

$$k \leqslant \begin{cases} n-3 & \text{if } n \text{ is even,} \\ n-2 & \text{if } n \text{ is odd.} \end{cases}$$

Note that for $n = 5$, Theorem 1 shows that exactly two ranks (1 and 3) occur among extreme rays of $\mathcal{D}_5$. Moreover for $X \in \text{Ext}(\mathcal{D}_5)$ it is obvious that $\text{rank}(X) = 1$ implies $X \in \mathcal{C}_5$. The converse is also true, because $X \in \mathcal{C}_5 \cap \text{Ext}(\mathcal{D}_5)$ implies $X \in \text{Ext}(\mathcal{C}_5)$, and therefore $\text{rank}(X) = 1$. So $X \in \text{Ext}(\mathcal{D}_5)$ with $\text{rank}(X) = 3$ must have $X \notin \mathcal{C}_5$, i.e., X is bad. The next result characterizes the rank-3 extreme rays of $\mathcal{D}_5$ via their graph structure.

Theorem 2. [8, Theorem 3.2] *Let $X \in \mathcal{D}_5$ with $\text{rank}(X) = 3$. Then $X \in \text{Ext}(\mathcal{D}_5)$ if and only if X is cyclic.*

Theorems 1 and 2 combine to yield the following characterization of extreme rays of $\mathcal{D}_5$.

Corollary 1. *Suppose $X \in \mathcal{D}_5$. Then $X \in \text{Ext}(\mathcal{D}_5)$ if and only if one of the following holds:*

(i) $\text{rank}(X) = 1$,
(ii) $\text{rank}(X) = 3$ *and X is cyclic.*

Moreover, (i) *implies $X \in \mathcal{C}_5$, while* (ii) *implies $X \notin \mathcal{C}_5$, i.e., X is bad.*

Motivated by Corollary 1, we define

$$\mathcal{E}_5 := \{X \in \text{Ext}(\mathcal{D}_5) : \text{rank}(X) = 3\} = \{X \in \mathcal{D}_5 : \text{rank}(X) = 3 \text{ and } X \text{ is cyclic}\}$$

to be the set of bad extreme rays of $\mathcal{D}_5$, which we will also refer to as *extremely bad* matrices in $\mathcal{D}_5$. Furthermore defining

$$\mathcal{B}_5 = \text{Cone}(\mathcal{E}_5),$$

it follows from Corollary 1 that

$$\mathcal{D}_5 = \mathcal{B}_5 + \mathcal{C}_5. \tag{1}$$

Given (1), an immediate consequence of Caratheodory's theorem is that any bad X can be written as the sum $X = Y + \sum_{j=1}^{15} Z_j$ for some $Y \in \mathcal{C}_5$ and $Z_1, \ldots, Z_{15} \in \mathcal{E}_5$. One of the main results of this paper (Corollary 2 in Section 4) is to show that this representation can be significantly streamlined. For bad X, we will prove in fact that $X = Y + Z$ for a *single* extremely bad Z. Moreover, this decomposition is computable (Algorithm 1).

At the end of the section we will demonstrate that the sets $\mathcal{B}_5$ and $\mathcal{C}_5$ have a nontrivial intersection; in particular, a sum of extremely bad 5×5 matrices can be CP. To do this we will utilize the following parameterization of matrices in $\mathcal{E}_5$ that will also be very useful in the analysis of Section 4.

Theorem 3. *$X \in \mathcal{E}_5$ if only if there exists a permutation matrix P, a positive diagonal matrix Λ, and a 5×3 matrix*

$$R = \begin{pmatrix} 1 & 0 & 0 \\ r_{21} & r_{22} & 1 \\ 0 & 1 & 0 \\ 0 & 1 & -r_{22} \\ 1 & 0 & -r_{21} \end{pmatrix} \quad (r_{21} > 0, r_{22} > 0)$$

such that $P^T XP = \Lambda RR^T \Lambda$.

Proof ($\Leftarrow$). The formula $P^T XP = \Lambda RR^T \Lambda$ shows $X \succeq 0$. Note also that the columns of R are linearly independent, so $\text{rank}(R) = 3$, which implies $\text{rank}(X) = 3$. Moreover,

$$\Lambda^{-1}P^TXP\Lambda^{-1} = RR^T = \begin{pmatrix} 1 & r_{21} & 0 & 0 & 1 \\ r_{21} & r_{21}^2 + r_{22}^2 + 1 & r_{22} & 0 & 0 \\ 0 & r_{22} & 1 & 1 & 0 \\ 0 & 0 & 1 & r_{22}^2 + 1 & r_{21}r_{22} \\ 1 & 0 & 0 & r_{21}r_{22} & r_{21}^2 + 1 \end{pmatrix}, \tag{2}$$

which demonstrates $X \geqslant 0$ and X cyclic.

[$\Rightarrow$] Because X is cyclic, under a suitable permutation P, P^TXP has the form

$$\begin{pmatrix} + & + & & & + \\ + & + & + & & \\ & + & + & + & \\ & & + & + & + \\ + & & & + & + \end{pmatrix}, \tag{3}$$

where a blank indicates a zero entry and a plus sign $(+)$ indicates a positive entry. Next, because $\text{rank}(X) = 3$, there exists some $\widehat{R} \in \mathbb{R}^{5\times 3}$ such that $P^TXP = \widehat{R}\widehat{R}^T$. Note that $\widehat{R}_{1\cdot} \neq 0$ and $\widehat{R}_{3\cdot} \neq 0$ are orthogonal due to (3). Let $Q \in \mathbb{R}^{3\times 3}$ be any orthogonal matrix such that $\widehat{R}_{1\cdot}Q$ and $\widehat{R}_{3\cdot}Q$ are positive multiples of $(1, 0, 0)$ and $(0, 1, 0)$, respectively, and $[\widehat{R}Q]_{23} \geqslant 0$. Define $\bar{R} := \widehat{R}Q$ so that $\bar{R}$ has the form

$$\bar{R} = \begin{pmatrix} \bar{r}_{11} & 0 & 0 \\ \bar{r}_{21} & \bar{r}_{22} & \bar{r}_{23} \\ 0 & \bar{r}_{32} & 0 \\ \bar{r}_{41} & \bar{r}_{42} & \bar{r}_{43} \\ \bar{r}_{51} & \bar{r}_{52} & \bar{r}_{53} \end{pmatrix} \quad (\bar{r}_{11}, \bar{r}_{32} > 0, \bar{r}_{23} \geqslant 0).$$

Note that $\bar{R}\bar{R}^T = \widehat{R}QQ^T\widehat{R}^T = \widehat{R}\widehat{R}^T = P^TXP$. The structure of (3) immediately implies $\bar{r}_{41} = \bar{r}_{52} = 0$ and $\bar{r}_{21}, \bar{r}_{51}, \bar{r}_{22}, \bar{r}_{42} > 0$, i.e.,

$$\bar{R} = \begin{pmatrix} \bar{r}_{11} & 0 & 0 \\ \bar{r}_{21} & \bar{r}_{22} & \bar{r}_{23} \\ 0 & \bar{r}_{32} & 0 \\ 0 & \bar{r}_{42} & \bar{r}_{43} \\ \bar{r}_{51} & 0 & \bar{r}_{53} \end{pmatrix} \quad (\bar{r}_{11}, \bar{r}_{21}, \bar{r}_{51}, \bar{r}_{22}, \bar{r}_{32}, \bar{r}_{42} > 0,\ \bar{r}_{23} \geqslant 0).$$

Now, $[P^TXP]_{42} = \bar{r}_{22}\bar{r}_{42} + \bar{r}_{23}\bar{r}_{43} = 0$ implies $\bar{r}_{23} > 0$ and $\bar{r}_{43} = -\bar{r}_{22}\bar{r}_{42}/\bar{r}_{23}$. Similarly, $\bar{r}_{53} = -\bar{r}_{21}\bar{r}_{51}/\bar{r}_{23}$. Hence,

$$\bar{R} = \begin{pmatrix} \bar{r}_{11} & 0 & 0 \\ \bar{r}_{21} & \bar{r}_{22} & \bar{r}_{23} \\ 0 & \bar{r}_{32} & 0 \\ 0 & \bar{r}_{42} & -\frac{\bar{r}_{22}\bar{r}_{42}}{\bar{r}_{23}} \\ \bar{r}_{51} & 0 & -\frac{\bar{r}_{21}\bar{r}_{51}}{\bar{r}_{23}} \end{pmatrix} \quad (\bar{r}_{ij} > 0). \tag{4}$$

The result of the theorem now follows by defining Λ via its diagonal entries $\lambda_1 := \bar{r}_{11}, \lambda_2 := \bar{r}_{23}, \lambda_3 := \bar{r}_{32}$, $\lambda_4 := \bar{r}_{42}$, and $\lambda_5 := \bar{r}_{51}$, and also defining $R := \Lambda^{-1}\bar{R}$. $\square$

The representation of Theorem 3 depends on matrices R, Λ, and P. We next argue that P can be limited to a subset of twelve 5×5 permutation matrices (out of the $5! = 120$ total). Our intent is both to simplify Theorem 3 conceptually and to simplify some of the technical details encountered in Section 4.

Given $X \in \mathcal{E}_5$, consider its cyclic graph $G(X)$, and let C be the canonical 5-cycle which connects 1–2–3–4–5–1. Note that Theorem 3 is based on permuting the rows and columns of X using some P so that P^TXP has the form in 3, i.e., $G(P^TXP) = C$. If two different permutations P_1 and P_2 both yield the canonical 5-cycle, i.e., if $G(P_1^TXP_1) = G(P_2^TXP_2) = C$, then Theorem 3 provides two different parameterizations of X. It is important to keep in mind that permuting to get C depends only on the nonzero pattern of X, not on the specific values of the nonzero entries. It follows that there is redundancy in the parameterization provided by Theorem 3 when *all* R, Λ, and P are considered.

There are a total of 12 undirected 5-cycles on the vertices $\{1, 2, 3, 4, 5\}$, and it not difficult to see that permutation is a group action on $\{1, 2, 3, 4, 5\}$. Moreover, this group action corresponds naturally to the action $G(X) \mapsto G(P^TXP)$. It follows that any cyclic $G(X)$ is taken to $G(P^TXP) = C$ by $120/12 = 10$ different permutation matrices P. In this sense, there are 12 different size-10 equivalence classes of permutation matrices, each taking a particular 5-cycle $G(X)$ to C. We stress again that these actions are irrespective of the actual values of nonzero entries of X.

It follows that the parameterization of Theorem 3 remains valid if we select a representative P from each equivalence class and restrict P to be one of these 12 representatives. (Note that there are different choices for the 12 representatives, but any specific choice will work for Theorem 3.) For example, it suffices to consider the permutation matrices corresponding to the following 12 permutation vectors π, where $\pi_i = k$ means that $P_{ik} = 1$:

$$\begin{matrix} (1,2,3,4,5), & (1,2,3,5,4), & (1,2,4,3,5), & (1,2,4,5,3), & (1,2,5,3,4), & (1,2,5,4,3), \\ (1,3,2,4,5), & (1,3,2,5,4), & (1,3,4,2,5), & (1,3,5,2,4), & (1,4,2,3,5), & (1,4,3,2,5). \end{matrix} \tag{5}$$

As an application of Theorem 3 we will now show that the cones $\mathcal{C}_5$ and $\mathcal{B}_5$ have a nontrivial intersection, as claimed above. Letting $P = I$, $\Lambda = I + 3e_3e_3^T$, and $r_{21} = r_{22} = 1$, we obtain the extremely bad matrix

$$X = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 3 & 4 & 0 & 0 \\ 0 & 4 & 16 & 4 & 0 \\ 0 & 0 & 4 & 2 & 1 \\ 1 & 0 & 0 & 1 & 2 \end{pmatrix}.$$

Let P_i, $i = 1, \ldots 5$, be the permutation matrices corresponding to the "shift" permutation vectors

$$(1,2,3,4,5), \quad (2,3,4,5,1), \quad (3,4,5,1,2), \quad (4,5,1,2,3), \quad (5,1,2,3,4),$$

and define $Y = \sum_{i=1}^{5} P_i^TXP_i$. Note that each of these permutations takes C to itself, so that $G(P_i^TXP_i) = C$ for all i. It is then obvious that each diagonal component of Y is the sum of the diagonal components of X, which is 24. Similarly each nonzero component above the diagonal of Y is the sum of the nonzero components above the diagonal of X, which is 11. Therefore

$$Y = \begin{pmatrix} 24 & 11 & 0 & 0 & 11 \\ 11 & 24 & 11 & 0 & 0 \\ 0 & 11 & 24 & 11 & 0 \\ 0 & 0 & 11 & 24 & 11 \\ 11 & 0 & 0 & 11 & 24 \end{pmatrix}.$$

Since Y is diagonally dominant, it is CP [2, Theorem 2.5], despite the fact that each $P_i^TXP_i$ is extremely bad.

3. A CP reduction procedure for $\mathcal{D}_n$

In this section we describe a procedure to, if possible, decompose a matrix $X \in \mathcal{D}_n$ into a sum $X = Y + Z$ with $0 \neq Y \in \mathcal{C}_n$ and $Z \in \mathcal{D}_n$. We think of the procedure as "reducing" X by removing the CP component Y.

Definition 1. A matrix $X \in \mathcal{D}_n$ is *CP-reducible* if there are $0 \neq Y \in \mathcal{C}_n$ and $Z \in \mathcal{D}_n$ so that $X = Y + Z$. If no such Y, Z exist, then X is *CP-irreducible*.

In particular, if X is CP-irreducible, then X is bad; however, some bad matrices are CP-reducible. In Section 4 we will show that, for $n = 5$, if X is CP-irreducible, then X is in fact extremely bad.

In Theorem 4 we give a checkable characterization for CP-reducibility of a matrix $X \in \mathcal{D}_n$. To prove the theorem we require the following two technical lemmas. (Lemma 1 will also be used in the proofs of Theorems 5 and 7.) The straightforward proofs are omitted; see also Exercises 1.7 and 1.17 of [2].

Lemma 1. *Let $A = UU^T$ where A is $n \times n$ and U is $n \times k$. Then* $\text{Range}(A) = \text{Range}(U)$.

Lemma 2. *Suppose $A, B \succeq 0$. Then there exists $\varepsilon > 0$ such that $A - \varepsilon B \succeq 0$ if and only if* $\text{Null}(A) \subseteq \text{Null}(B)$, *which is equivalent to* $\text{Range}(B) \subseteq \text{Range}(A)$. *In particular, for $f \in \mathbb{R}^n$, there exists $\varepsilon > 0$ such that $A - \varepsilon ff^T \succeq 0$ if and only if $f \in$* $\text{Range}(A)$.

Theorem 4. *Let $X \in \mathcal{D}_n$. Then X is CP-reducible if and only if there exists a partition (I, J) of $\{1, \ldots, n\}$ such that $I \neq \emptyset, X_{II} > 0$, and there is an $f \in$ Range(X) with $f \geqslant 0, f_J = 0, f_I \neq 0$.*

Proof ($\Leftarrow$). Suppose that $I \neq \emptyset, X_{II} > 0, f \in \text{Range}(X), f \geqslant 0, f_J = 0, f_I \neq 0$. Then by Lemma 2 there exists $\varepsilon > 0$ such that $Z(\varepsilon) := X - \varepsilon ff^T \succeq 0$. Because $f_J = 0$, we have

$$[Z(\varepsilon)]_{II} = X_{II} - \varepsilon f_I f_I^T, \quad [Z(\varepsilon)]_{IJ} = X_{IJ}, \quad [Z(\varepsilon)]_{JJ} = X_{JJ}.$$

Hence, because $X \geqslant 0$ and $X_{II} > 0$, there is an $\varepsilon > 0$ such that $Z(\varepsilon) \in \mathcal{D}_n$. Take $Z := Z(\varepsilon)$ and $Y = \varepsilon ff^T$.

[$\Rightarrow$] Assume that $X = Y + Z$, where $Y = NN^T \neq 0$ with $N \geqslant 0$. Let $f \geqslant 0$ be any nonzero column of N. Let $I := \{i : f_i > 0\}$. Clearly $X_{II} > 0$, and $X - ff^T \in \mathcal{D}_n$. Lemma 2 then implies $f \in \text{Range}(X)$. $\square$

For any $I \subseteq \{1, \ldots, n\}$, the conditions in Theorem 4 can be checked by solving the linear programming problem

$$\begin{aligned} \max \quad & e^T f \\ \text{s.t.} \quad & Xw = f, \quad e^T f \leqslant 1, \\ & f \geqslant 0, \quad f_J = 0, \quad w \text{ free}. \end{aligned} \tag{6}$$

Note that the constraint $e^T f \leqslant 1$ is used only to bound the feasible set of the problem. As such, the optimal value of (6) equals either 0 or 1. Let f^* be an optimal solution of (6). If $e^T f^* = 1$, then X is CP-reducible, and one may take $Y := \varepsilon^* f^* (f^*)^T$ and $Z := X - \varepsilon^* f^* (f^*)^T$, where $\varepsilon^* = \max\{\varepsilon > 0 : X - \varepsilon f^* (f^*)^T \in \mathcal{D}_n\}$. On the other hand if the solution value of (6) is zero for every I then we have a proof that X is CP-irreducible by Theorem 4. Repeated application of this procedure results in the CP reduction algorithm given in Algorithm 1. Finiteness of Algorithm 1 is established in Theorem 5, below.

Algorithm 1: CP Reduction of a DNN Matrix

Input $X \in \mathcal{D}_n$
1: Set $Y_0 := 0$ and $Z_0 := X$.
2: **for** $k = 0, 1, 2, \ldots$
3: Find a partition (I, J) of $\{1, \ldots, n\}$ such that:
 (i) $I \neq \emptyset$,
 (ii) $[Z_k]_{II} > 0$,
 (iii) the optimal value of (6) – with X replaced by Z_k – is 1. Let f_k be an optimal solution of (6).
 If no such partition (I, J) is found, then set $Y := Y_k, Z := Z_k$ and STOP.
4: Let ε_k be the optimal value of $\max\{\varepsilon > 0 : Z_k - \varepsilon f_k f_k^T \in \mathcal{D}_n\}$.
5: Set $Y_{k+1} := Y_k + \varepsilon_k f_k f_k^T$ and $Z_{k+1} := Z_k - \varepsilon_k f_k f_k^T$.
6: **end for**
Output A decomposition $X = Y + Z$ where $Y \in \mathcal{C}_n, Z \in \mathcal{D}_n$ and Z is CP-irreducible.

We illustrate the behavior of Algorithm 1 with one iteration on the following example. Consider the completely positive matrix $X = NN^T$ with

$$N = \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 2 \\ 1 & 1 & 0 & 0 & 0 & 2 & 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 2 & 1 \end{pmatrix}, \quad \text{i.e., } X = \begin{pmatrix} 8 & 5 & 1 & 1 & 5 \\ 5 & 8 & 5 & 1 & 1 \\ 1 & 5 & 8 & 5 & 1 \\ 1 & 1 & 5 & 8 & 5 \\ 5 & 1 & 1 & 5 & 8 \end{pmatrix}.$$

The decomposition produced by one iteration of Algorithm 1 depends on the choice of partition (I, J) in Step 3. If we take $I = \{1, \ldots, 5\}$, the solution of (6) is $f^* = \frac{1}{5}e$. Step 1 then gives $\varepsilon_0 = 25$, so we get the decomposition $X = Y_1 + Z_1$ with $Y_1 = ee^T$ and

$$Z_1 = \begin{pmatrix} 7 & 4 & 0 & 0 & 4 \\ 4 & 7 & 4 & 0 & 0 \\ 0 & 4 & 7 & 4 & 0 \\ 0 & 0 & 4 & 7 & 4 \\ 4 & 0 & 0 & 4 & 7 \end{pmatrix}.$$

Note that $Z_1 \in \mathcal{D}_5$, but Z_1 is a bad matrix, i.e., $Z_1 \notin \mathcal{C}_5$, because $Z_1 \bullet H = -5 < 0$ for the copositive Horn matrix

$$H := \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}. \tag{7}$$

The matrix H was first proposed by Horn, cf. [7], who showed that H is a copositive matrix which can not be represented as the sum of a positive semidefinite and a nonnegative matrix, i.e., $H \in \mathcal{C}_5^* \setminus \mathcal{D}_5^*$.

Note that a byproduct of Algorithm 1 is a CP representation of the output Y, which is built up as the sum of the rank-1 CP matrices $\varepsilon_k f_k f_k^T$, one per iteration. A reasonable question to ask is whether Algorithm 1 necessarily generates a CP representation NN^T of X, when the input X is CP. Said differently, for $X \in \mathcal{C}_n$, does Algorithm 1 guarantee output $(Y, Z) = (X, 0)$? The example X just considered shows that this is not the case. Indeed, since $Z_1 \notin \mathcal{C}_5$, the remaining iterations of Algorithm 1 cannot produce a CP factorization of X because otherwise we would also have a CP factorization of Z_1. In particular, the algorithm does *not* reproduce the original factorization $X = NN^T$. One might suspect that a different, more intelligent initial choice for I in Algorithm 1 might enable $(Y, Z) = (X, 0)$. However, even if we take I to be the support of one of the columns of N, we observe the same phenomenon. For example, take $I = \{1, 2, 3\}$, the support of the sixth column of N. Then the solution of (6) is $f = (0.4710, 0.0580, 0.4710, 0, 0)^T$, which is not a multiple of $N_{\cdot 6}$. Step 1 gives $\varepsilon_0 = 2.5584$, and again $Z_1 = X - \varepsilon_0 ff^T$ is a bad matrix, since $Z_1 \bullet H = -1.9995 < 0$.

So Algorithm 1 in general produces a decomposition $X = Y + Z$ with $0 \neq Z \in \mathcal{D}_n$, even if the input matrix X is completely positive. This is not so surprising given that the problem of determining whether or not a given DNN matrix is CP appears to be quite difficult [1,13]. Even with this limitation, we show in the next section that Algorithm 1 has very useful properties when applied to an initial matrix X in $\mathcal{D}_5 \setminus \mathcal{C}_5$. As promised earlier, the next theorem shows that Algorithm 1 is a finite procedure.

Theorem 5. *Given input $X \in \mathcal{D}_n$, Algorithm 1 terminates after at most $n + n(n+1)/2$ iterations with an output decomposition $X = Y + Z$ where $Y \in \mathcal{C}_n$, $Z \in \mathcal{D}_n$ and Z is CP-irreducible.*

Proof. For a symmetric matrix M, let $\mathrm{nz}(M)$ denote the number of nonzeros on or above the diagonal of M. We claim that, for each k, either $\mathrm{rank}(Z_{k+1}) < \mathrm{rank}(Z_k)$ or $\mathrm{nz}(Z_{k+1}) < \mathrm{nz}(Z_k)$.

Suppose the line search $Z_k - \varepsilon f_k f_k^T$ in Step 1 of Algorithm 1 is limited by $Z_k - \varepsilon f_k f_k^T \geqslant 0$. Then $\mathrm{nz}(Z_{k+1}) < \mathrm{nz}(Z_k)$. On the other hand, suppose it is limited by $Z_k - \varepsilon f_k f_k^T \succeq 0$. Let $Z_k = UU^T$, where the number of columns of U is $\mathrm{rank}(Z_k)$. The condition $f_k \in \mathrm{Range}(Z_k)$ implies $f_k \in \mathrm{Range}(U)$, since both sets are equal by Lemma 1, so let y satisfy $f_k = Uy$. Then the factorization

$$Z_k - \varepsilon f_k f_k^T = UU^T - \varepsilon Uyy^T U^T = U(I - \varepsilon yy^T)U^T$$

shows that the line search is limited by $I - \varepsilon yy^T \succeq 0$. Said differently, ε_k yields $\text{rank}(I - \varepsilon_k yy^T) \leqslant \text{rank}(Z_k) - 1$. Hence, $\text{rank}(Z_{k+1}) < \text{rank}(Z_k)$. Moreover, both $\text{rank}(Z_k)$ and $\text{nz}(Z_k)$ are clearly nonnegative and nonincreasing, so $\text{rank}(Z_k) + \text{nz}(Z_k) \leqslant n + n(n+1)/2$ strictly decreases in every iteration, and is 0 if and only if $Z_k = 0$ (in which case the algorithm clearly stops). The fact that the matrix Z in the decomposition $X = Y + Z$ produced by Algorithm 1 is CP-irreducible follows immediately from Theorem 4. □

Observe that Theorem 5 does *not* imply that Algorithm 1 is a polynomial time algorithm. Although each problem of the form (6) can be solved in polynomial time and the number of iterations is polynomial, Step 1 is not, since in the worst case an exponential number of possible partitions of $\{1, \ldots, n\}$ must be tested.

4. The CP reduction applied to $\mathcal{D}_5$

In this section we will show that a 5×5 CP-irreducible matrix, as output by Algorithm 1 when applied to an input matrix in $\mathcal{D}_5$, must in fact be extremely bad. We will repeatedly use the following simple property of CP-reducibility for the sum of two matrices in $\mathcal{D}_n$.

Lemma 3. *Assume that $X_1, X_2 \in \mathcal{D}_n$. Then the following three conditions are equivalent*:

(i) *$X_1 + X_2$ is CP-reducible,*
(ii) *$\alpha_1 X_1 + \alpha_2 X_2$ is CP-reducible for some $\alpha_1, \alpha_2 > 0$,*
(iii) *$\alpha_1 X_1 + \alpha_2 X_2$ is CP-reducible for all $\alpha_1, \alpha_2 > 0$.*

Proof. Obviously (iii) $\Rightarrow$ (i) $\Rightarrow$ (ii). To show that (ii) $\Rightarrow$ (iii), assume that $\alpha_1 X_1 + \alpha_2 X_2$ is CP-reducible and we want to show that $\beta_1 X_1 + \beta_2 X_2$ is CP-reducible. Assume w.l.o.g. that $\beta_2/\alpha_2 \geq \beta_1/\alpha_1$ (otherwise interchange the indices). Note that

$$\begin{aligned}\beta_1 X_1 + \beta_2 X_2 &= \frac{\beta_1}{\alpha_1}(\alpha_1 X_1 + \alpha_2 X_2) + \left(\beta_2 - \frac{\beta_1 \alpha_2}{\alpha_1}\right) X_2 \\ &= \frac{\beta_1}{\alpha_1}(Y + Z) + \alpha_2 \left(\frac{\beta_2}{\alpha_2} - \frac{\beta_1}{\alpha_1}\right) X_2,\end{aligned}$$

where $0 \neq Y \in \mathcal{C}_n$ and $Z \in \mathcal{D}_n$, since $\alpha_1 X_1 + \alpha_2 X_2$ is CP-reducible. Therefore $\beta_1 X_1 + \beta_2 X_2$ is also CP-reducible, as required. □

It is obvious, for example from (1), that if a matrix $Z \in \mathcal{D}_5$ is CP-irreducible, then there are matrices $\{X_i\}_{i=1}^k$, where $k \leqslant 15$ and each $X_i \in \mathcal{E}_5$, so that $Z = \sum_{i=1}^k X_i$. Applying Theorem 3 we can then write Z in the form

$$Z = \sum_{i=1}^k P_i^T \Lambda_i R_i R_i^T \Lambda_i P_i, \tag{8}$$

where each P_i is a permutation matrix corresponding to one of the permutation vectors in (5) and each pair (Λ_i, R_i) has the form given in Theorem 3. Our goal is to show that if Z is CP-irreducible, then in fact $k = 1$ in (8). We will first show that if two terms in (8) have $P_i \neq P_j$, then Z is CP-reducible.

Theorem 6. *Let $n = 5$, and assume that $U = P_1^T \Lambda R R^T \Lambda P_1$, $V = P_2^T \Theta S S^T \Theta P_2$ where (Λ, R) and (Θ, S) have the form given in Theorem 3 and $P_1 \neq P_2$ are permutation matrices. Then $U + V$ is CP-reducible.*

Proof. We may assume w.l.o.g. that $P_1 = I$ and consider cases corresponding to P_2 associated with one of the permutation vectors π from (5) other than $(1, 2, 3, 4, 5)$.

To begin, consider $\pi = (1, 3, 5, 2, 4)$. Then $G(V)$ is the cycle 1–3–5–2–4–1, which is the complement of the cycle 1–2–3–4–5–1. It follows that $X = U + V > 0$, so setting f equal to any column of X satisfies the conditions of Theorem 4, with $J = \emptyset$. Therefore $U + V$ is CP-reducible.

Next consider $\pi = (1, 4, 2, 3, 5)$. By Lemma 3, to show that $U + V$ is CP-reducible it suffices to show that $X(\varepsilon) := U + \varepsilon V$ is CP-reducible for some $\varepsilon > 0$, where

$$X(\varepsilon) = \begin{pmatrix} u_{11}+\varepsilon v_{11} & u_{12} & 0 & \varepsilon v_{14} & u_{15}+\varepsilon v_{15} \\ u_{21} & u_{22}+\varepsilon v_{22} & u_{23}+\varepsilon v_{23} & \varepsilon v_{24} & 0 \\ 0 & u_{32}+\varepsilon v_{32} & u_{33}+\varepsilon v_{33} & u_{34} & \varepsilon v_{35} \\ \varepsilon v_{41} & \varepsilon v_{42} & u_{43} & u_{44}+\varepsilon v_{44} & u_{45} \\ u_{51}+\varepsilon v_{51} & 0 & \varepsilon v_{53} & u_{54} & u_{55}+\varepsilon v_{55} \end{pmatrix}.$$

Note that for $J = \{1, 2\}$, we have $X(\varepsilon)_{JJ} > 0$ for any $\varepsilon > 0$. In addition, the vector

$$f(\varepsilon) := X(\varepsilon)_{\cdot 4} - \frac{\varepsilon v_{24}}{u_{23}+\varepsilon v_{23}} X(\varepsilon)_{\cdot 3} - \frac{\varepsilon v_{14}}{u_{15}+\varepsilon v_{15}} X(\varepsilon)_{\cdot 5}$$

has $f(\varepsilon)_J = 0$, and $f(\varepsilon)_I > 0$ for all $\varepsilon > 0$ sufficiently small. It follows from Theorem 4 that $X(\varepsilon) = U + \varepsilon V$ is CP-reducible for all $\varepsilon > 0$ sufficiently small. A similar argument applies for the permutation vectors $(1, 2, 5, 3, 4)$, $(1, 3, 2, 5, 4)$, $(1, 3, 4, 2, 5)$ and $(1, 2, 4, 5, 3)$, with the index set $J = \{1, 2\}$ replaced by $\{2, 3\}$, $\{3, 4\}$, $\{4, 5\}$ and $\{5, 1\}$, respectively.

Finally consider $\pi = (1, 2, 4, 3, 5)$. We again define $X(\varepsilon) = U + \varepsilon V$, which now has the form

$$X(\varepsilon) = \begin{pmatrix} u_{11}+\varepsilon v_{11} & u_{12}+\varepsilon v_{12} & 0 & 0 & u_{15}+\varepsilon v_{15} \\ u_{21}+\varepsilon v_{21} & u_{22}+\varepsilon v_{22} & u_{23} & \varepsilon v_{24} & 0 \\ 0 & u_{32} & u_{33}+\varepsilon v_{33} & u_{34}+\varepsilon v_{34} & \varepsilon v_{35} \\ 0 & \varepsilon v_{42} & u_{43}+\varepsilon v_{43} & u_{44}+\varepsilon v_{44} & u_{45} \\ u_{51}+\varepsilon v_{51} & 0 & \varepsilon v_{53} & u_{54} & u_{55}+\varepsilon v_{55} \end{pmatrix}.$$

For $J = \{1, 2\}$, we again have $X(\varepsilon)_{JJ} > 0$ for any $\varepsilon > 0$. In addition, the vector

$$f(\varepsilon) := X(\varepsilon)_{\cdot 4} - \frac{\varepsilon v_{24}}{u_{23}} X(\varepsilon)_{\cdot 3}$$

has $f(\varepsilon)_J = 0$, and $f(\varepsilon)_I > 0$ for all $\varepsilon > 0$ sufficiently small. It follows from Theorem 4 that $X(\varepsilon) = U + \varepsilon V$ is CP-reducible for all $\varepsilon > 0$ sufficiently small. A similar argument applies for the permutation vectors $(1, 2, 3, 5, 4)$, $(1, 4, 3, 2, 5)$, $(1, 2, 5, 4, 3)$ and $(1, 3, 2, 4, 5)$, with the index set $J = \{1, 2\}$ replaced by $\{2, 3\}$, $\{3, 4\}$, $\{4, 5\}$ and $\{5, 1\}$, respectively. $\square$

By Theorem 6, if Z given in (8) is CP-irreducible then it must be that $P_i = P_j$ for all i, j. Moreover, when $P_i = P_j$ we may assume that $\Lambda_j R_j$ is not a multiple of $\Lambda_i R_i$, since otherwise the two terms can be combined. We will next show that if $P_i = P_j$ but $\Lambda_j R_j$ is not a multiple of $\Lambda_i R_i$, then Z is CP-reducible.

Theorem 7. *Let $n = 5$, and assume that $U = P^T \Lambda R R^T \Lambda P$, $V = P^T \Theta S S^T \Theta P$ where (Λ, R) and (Θ, S) have the form given in Theorem 3, P is a permutation matrix, and ΘS is not a multiple of ΛR. Then $U + V$ is CP-reducible.*

Proof. We may assume w.l.o.g. that $P = I$. By Theorem 4, $U + V$ is CP-reducible if and only if there is an index set $I \neq \emptyset$ so that $(U + V)_{II} > 0$ and the system

$$\begin{aligned} & e^T f \geqslant 1, \\ & (U+V)w = f, \\ & f \geqslant 0, \quad f_J = 0 \end{aligned} \tag{9}$$

is feasible. Let $\bar{R} = \Lambda R$, $\bar{S} = \Theta S$. Since $U + V = \bar{R}\bar{R}^T + \bar{S}\bar{S}^T = (\bar{R}, \bar{S})(\bar{R}, \bar{S})^T$, we may apply Lemma 1 and conclude that (9) is feasible if and only if the system

$$\begin{aligned}&\overline{R}_{I\cdot}u+\overline{S}_{I\cdot}v\geqslant 0,\\&\overline{R}_{J\cdot}u+\overline{S}_{J\cdot}v=0,\\&e^T\overline{R}_{I\cdot}u+e^T\overline{S}_{I\cdot}v\geqslant 1\end{aligned}\tag{10}$$

is feasible. Thus to show that $U+V$ is CP-reducible it suffices to show that (10) is feasible for some $I\neq\emptyset$. We will show that if (10) is infeasible for both $I=\{1,2\}$ and $I=\{1,5\}$, then $\overline{S}$ must be a multiple of $\overline{R}$.

By Farkas' lemma, for a given I the system (10) is infeasible if and only if the system

$$\begin{aligned}&x^T\overline{R}_{I\cdot}+z^T\overline{R}_{J\cdot}+e^T\overline{R}_{I\cdot}=0,\\&x^T\overline{S}_{I\cdot}+z^T\overline{S}_{J\cdot}+e^T\overline{S}_{I\cdot}=0,\\&x\geqslant 0,\quad z\text{ free}\end{aligned}\tag{11}$$

is feasible. It is easy to check that for both I under consideration, $\overline{R}_{J\cdot}$ and $\overline{S}_{J\cdot}$ are always invertible. Using this fact, (11) can be rewritten as

$$\begin{aligned}&(x+e)^T\overline{R}_{I\cdot}\overline{R}_{J\cdot}^{-1}=z,\\&(x+e)^T\overline{S}_{I\cdot}\overline{S}_{J\cdot}^{-1}=z,\\&x\geqslant 0,\quad z\text{ free},\end{aligned}$$

which is equivalent to

$$x^T\left(\overline{R}_{I\cdot}\overline{R}_{J\cdot}^{-1}-\overline{S}_{I\cdot}\overline{S}_{J\cdot}^{-1}\right)=0,\qquad x>0.\tag{12}$$

We will consider (12) in detail for $I=\{1,2\}$ and $I=\{1,5\}$. We use the form of $\overline{R}$ (which similarly holds for $\overline{S}$) given in 4. For $I=\{1,2\}$ it is straightforward to compute that

$$\overline{R}_{I\cdot}\overline{R}_{J\cdot}^{-1}=\begin{pmatrix}\frac{\bar r_{11}\bar r_{21}}{\bar r_{22}\bar r_{32}} & -\frac{\bar r_{11}\bar r_{21}}{\bar r_{22}\bar r_{42}} & \frac{\bar r_{11}}{\bar r_{51}}\\ \frac{\bar r_{21}^2+\bar r_{22}^2+\bar r_{23}^2}{\bar r_{22}\bar r_{32}} & -\frac{\bar r_{21}^2+\bar r_{23}^2}{\bar r_{22}\bar r_{42}} & \frac{\bar r_{21}}{\bar r_{51}}\end{pmatrix},\tag{13}$$

and $\overline{S}_{I\cdot}\overline{S}_{J\cdot}^{-1}$ has the same form, with $\bar s_{ij}$ replacing $\bar r_{ij}$ throughout. For $I=\{1,5\}$ it is straightforward to compute that

$$\overline{R}_{I\cdot}\overline{R}_{J\cdot}^{-1}=\begin{pmatrix}\frac{\bar r_{11}}{\bar r_{21}} & -\frac{\bar r_{11}(\bar r_{22}^2+\bar r_{23}^2)}{\bar r_{21}\bar r_{22}\bar r_{32}} & \frac{\bar r_{11}\bar r_{23}^2}{\bar r_{21}\bar r_{22}\bar r_{42}}\\ \frac{\bar r_{51}}{\bar r_{21}} & -\frac{\bar r_{51}(\bar r_{21}^2+\bar r_{22}^2+\bar r_{23}^2)}{\bar r_{21}\bar r_{22}\bar r_{32}} & \frac{\bar r_{51}(\bar r_{21}^2+\bar r_{23}^2)}{\bar r_{21}\bar r_{22}\bar r_{42}}\end{pmatrix},\tag{14}$$

and $\overline{S}_{I\cdot}\overline{S}_{J\cdot}^{-1}$ has the same form, with $\bar s_{ij}$ replacing $\bar r_{ij}$ throughout. Recall that by Lemma 3, $U+V$ is CP-irreducible if and only if $\alpha U+\beta V$ is CP-irreducible for any $\alpha,\ \beta>0$, and therefore we are free to scale $\overline{R}$ and $\overline{S}$ by any positive factors. For convenience we scale $\overline{R}$ by $1/\bar r_{51}$ and $\overline{S}$ by $1/\bar s_{51}$, so henceforth we assume that $\bar r_{51}=\bar s_{51}=1$. Our goal is then to show that if (12) is feasible for $I=\{1,2\}$ and $I=\{1,5\}$, it must be that $\overline{R}=\overline{S}$.

To begin, for $I=\{1,2\}$, (12) and the third column of (13) implies that there is an $x>0$ such that

$$x^T\begin{pmatrix}\bar r_{11}-\bar s_{11}\\ \bar r_{21}-\bar s_{21}\end{pmatrix}=0,\tag{15}$$

while for $I=\{1,5\}$, (12) and the first column of (14) (with denominators cleared) implies that there is a $y>0$ such that

$$y^T\begin{pmatrix}\bar r_{11}\bar s_{21}-\bar s_{11}\bar r_{21}\\ \bar s_{21}-\bar r_{21}\end{pmatrix}=0.\tag{16}$$

Assume for the moment that $\bar r_{11}>\bar s_{11}$. Then (15) implies that $\bar s_{21}>\bar r_{21}$, so $\bar r_{11}\bar s_{21}>\bar s_{11}\bar r_{21}$ also, which is impossible by (16). A similar contradiction results from the assumption that $\bar r_{11}<\bar s_{11}$. Therefore $\bar r_{11}=\bar s_{11}$, and (15) implies that $\bar r_{21}=\bar s_{21}$ as well.

Next, for $I = \{1, 2\}$, (12) and the second column of (13) (multiplied by -1 and with denominators cleared), along with the facts that $\bar{r}_{11} = \bar{s}_{11}$ and $\bar{r}_{21} = \bar{s}_{21}$, implies that there is an $x > 0$ with

$$x^T \begin{pmatrix} \bar{r}_{11}\bar{r}_{21} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \bar{s}_{22}\bar{s}_{42} - \bar{r}_{22}\bar{r}_{42} \\ \bar{r}_{21}^2(\bar{s}_{22}\bar{s}_{42} - \bar{r}_{22}\bar{r}_{42}) + \bar{s}_{22}\bar{s}_{42}\bar{r}_{23}^2 - \bar{r}_{22}\bar{r}_{42}\bar{s}_{23}^2 \end{pmatrix} = 0, \tag{17}$$

while for $I = \{1, 5\}$, (12) and the third column of (14) (with denominators cleared) implies that there is a $y > 0$ such that

$$y^T \begin{pmatrix} \bar{r}_{11} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \bar{s}_{22}\bar{s}_{42}\bar{r}_{23}^2 - \bar{r}_{22}\bar{r}_{42}\bar{s}_{23}^2 \\ \bar{r}_{21}^2(\bar{s}_{22}\bar{s}_{42} - \bar{r}_{22}\bar{r}_{42}) + \bar{s}_{22}\bar{s}_{42}\bar{r}_{23}^2 - \bar{r}_{22}\bar{r}_{42}\bar{s}_{23}^2 \end{pmatrix} = 0. \tag{18}$$

Assume for the moment that $\bar{s}_{22}\bar{s}_{42} - \bar{r}_{22}\bar{r}_{42} > 0$. Then (17) implies that $\bar{r}_{21}^2(\bar{s}_{22}\bar{s}_{42} - \bar{r}_{22}\bar{r}_{42}) + \bar{s}_{22}\bar{s}_{42}\bar{r}_{23}^2 - \bar{r}_{22}\bar{r}_{42}\bar{s}_{23}^2 < 0$ and therefore $\bar{s}_{22}\bar{s}_{42}\bar{r}_{23}^2 - \bar{r}_{22}\bar{r}_{42}\bar{s}_{23}^2 < 0$ as well, which is impossible by (18). Assuming that $\bar{s}_{22}\bar{s}_{42} - \bar{r}_{22}\bar{r}_{42} < 0$ leads to a similar contradiction. Therefore we must have $\bar{r}_{22}\bar{r}_{42} = \bar{s}_{22}\bar{s}_{42}$, and $\bar{r}_{23} = \bar{s}_{23}$ follows immediately from (17).

Finally, for $I = \{1, 2\}$, (12) and the first column of (13) (with denominators cleared) along with the facts that $\bar{r}_{11} = \bar{s}_{11}$, $\bar{r}_{21} = \bar{s}_{21}$ and $\bar{r}_{23} = \bar{s}_{23}$ implies that there is an $x > 0$ with

$$x^T \begin{pmatrix} \bar{r}_{11}\bar{r}_{21} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \bar{s}_{22}\bar{s}_{32} - \bar{r}_{22}\bar{r}_{32} \\ (\bar{r}_{21}^2 + \bar{r}_{23}^2)(\bar{s}_{22}\bar{s}_{32} - \bar{r}_{22}\bar{r}_{32}) + \bar{r}_{22}\bar{s}_{22}(\bar{r}_{22}\bar{s}_{32} - \bar{s}_{22}\bar{r}_{32}) \end{pmatrix} = 0, \tag{19}$$

while for $I = \{1, 5\}$, (12) and the second column of (14) (multiplied by -1 and with denominators cleared) implies that there is a $y > 0$ such that

$$y^T \begin{pmatrix} \bar{r}_{11} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \bar{r}_{23}^2(\bar{s}_{22}\bar{s}_{32} - \bar{r}_{22}\bar{r}_{32}) + \bar{r}_{22}\bar{s}_{22}(\bar{r}_{22}\bar{s}_{32} - \bar{s}_{22}\bar{r}_{32}) \\ (\bar{r}_{21}^2 + \bar{r}_{23}^2)(\bar{s}_{22}\bar{s}_{32} - \bar{r}_{22}\bar{r}_{32}) + \bar{r}_{22}\bar{s}_{22}(\bar{r}_{22}\bar{s}_{32} - \bar{s}_{22}\bar{r}_{32}) \end{pmatrix} = 0. \tag{20}$$

Assume for the moment that $\bar{s}_{22}\bar{s}_{32} - \bar{r}_{22}\bar{r}_{32} > 0$. Then (19) implies that $(\bar{r}_{21}^2 + \bar{r}_{23}^2)(\bar{s}_{22}\bar{s}_{32} - \bar{r}_{22}\bar{r}_{32}) + \bar{r}_{22}\bar{s}_{22}(\bar{r}_{22}\bar{s}_{32} - \bar{s}_{22}\bar{r}_{32}) < 0$, and therefore $\bar{r}_{23}^2(\bar{s}_{22}\bar{s}_{32} - \bar{r}_{22}\bar{r}_{32}) + \bar{r}_{22}\bar{s}_{22}(\bar{r}_{22}\bar{s}_{32} - \bar{s}_{22}\bar{r}_{32}) < 0$ as well, which is impossible by (20). Assuming that $\bar{s}_{22}\bar{s}_{32} - \bar{r}_{22}\bar{r}_{32} < 0$ produces a similar contradiction, and therefore we must have $\bar{r}_{22}\bar{r}_{32} = \bar{s}_{22}\bar{s}_{32}$. Then $\bar{r}_{22} = \bar{s}_{22}$ follows from (19), and from $\bar{r}_{22}\bar{r}_{32} = \bar{s}_{22}\bar{s}_{32}$ and $\bar{r}_{22}\bar{r}_{42} = \bar{s}_{22}\bar{s}_{42}$ we obtain $\bar{r}_{32} = \bar{s}_{32}$ and $\bar{r}_{42} = \bar{s}_{42}$. We have thus shown that $\bar{R} = \bar{S}$, as required. □

Combining Theorems 5, 6 and 7 with the obvious fact that an extremely bad matrix is CP-irreducible, we obtain the desired final result.

Corollary 2. *Let $X \in \mathcal{D}_5$. Then X is CP-irreducible if and only if X is extremely bad. Moreover, if $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ then there are $Y \in \mathcal{C}_5$ and $Z \in \mathcal{E}_5$ so that $X = Y + Z$.*

5. Separating a rank-3 extreme ray of $\mathcal{D}_5$ from $\mathcal{C}_5$

A natural question arising in the context of optimization over the cone $\mathcal{C}_5$ is whether or not it is possible to *separate* a given bad matrix X from $\mathcal{C}_5$. Said differently, we look for a linear inequality that is valid for all $Y \in \mathcal{C}_5$, but which is not satisfied by $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$. We have not been able to derive a separating inequality for an arbitrary bad matrix, but we show below how to separate an extremely bad matrix $X \in \mathcal{E}_5$ from $\mathcal{C}_5$. The matrix H in the statement of Lemma 4 and Theorem 8 is the Horn matrix from (7).

Lemma 4. *Let $X \in \mathrm{Ext}(\mathcal{D}_5)$ be a cyclic matrix with $\mathrm{rank}(X) = 3$, and let $P^T X P = \Lambda R R^T \Lambda$ be its representation provided by Theorem 3. Then*

(i) *$P^T XP \circ H$ is invertible*;
(ii) *$(P^T XP \circ H)^{-1} e < 0$.*

Proof. To prove (i), since $P^TXP \circ H = \Lambda(RR^T \circ H)\Lambda$, it suffices to show that $RR^T \circ H$ is invertible. Using the parameterized form (2) of RR^T from the proof of Theorem 3, it is easy to verify that

$$(RR^T \circ H)^{-1} = -\frac{1}{2}\begin{pmatrix} 0 & \frac{1}{r_{21}} & \frac{r_{21}^2+r_{22}^2+1}{r_{21}r_{22}} & \frac{r_{21}^2+1}{r_{21}r_{22}} & 1 \\ \frac{1}{r_{21}} & 0 & \frac{1}{r_{22}} & \frac{1}{r_{22}} & \frac{1}{r_{21}} \\ \frac{r_{21}^2+r_{22}^2+1}{r_{21}r_{22}} & \frac{1}{r_{22}} & 0 & 1 & \frac{r_{22}^2+1}{r_{21}r_{22}} \\ \frac{r_{21}^2+1}{r_{21}r_{22}} & \frac{1}{r_{22}} & 1 & 0 & \frac{1}{r_{21}r_{22}} \\ 1 & \frac{1}{r_{21}} & \frac{r_{22}^2+1}{r_{21}r_{22}} & \frac{1}{r_{21}r_{22}} & 0 \end{pmatrix},$$

which proves (i). Note that all off-diagonal entries of $(RR^T \circ H)^{-1}$ are negative, which implies that all off-diagonal entries of $(P^TXP \circ H)^{-1} = \Lambda^{-1}(RR^T \circ H)^{-1}\Lambda^{-1}$ are also negative. This proves (ii). □

Theorem 8. *Let $X \in \mathrm{Ext}(\mathcal{D}_5)$ be a cyclic matrix with $\mathrm{rank}(X) = 3$, and let $P^TXP = \Lambda RR^T\Lambda$ be its representation provided by Theorem 3. Define $w := -(P^TXP \circ H)^{-1}e$ and $K := P\mathrm{Diag}(w)H\mathrm{Diag}(w)P^T$. Then the hyperplane $\{Y \in S_5 : K \bullet Y = 0\}$ separates X from $\mathcal{C}_5$; that is, $K \bullet Y \geqslant 0$ for all $Y \in \mathcal{C}_5$, but $K \bullet X < 0$. Moreover, the cut is sharp in the sense that there is $\widehat{Y} \in \mathcal{C}_5$ with $K \bullet \widehat{Y} = 0$.*

Proof. First note that $(P^TXP \circ H)^{-1}$ exists and $w > 0$ by Lemma 4. Also, $K \in \mathcal{C}_5^*$ (the cone of 5×5 copositive matrices) because $w > 0$ and $H \in \mathcal{C}_5^*$. Hence, $K \bullet Y \geqslant 0$ for all $Y \in \mathcal{C}_5$ (note that $P^T\mathcal{C}_5P = \mathcal{C}_5$). Moreover

$$\begin{aligned} K \bullet X &= \mathrm{Diag}(w)H\mathrm{Diag}(w) \bullet P^TXP \\ &= (H \circ ww^T) \bullet P^TXP = ww^T \bullet (P^TXP \circ H) \\ &= w^T(P^TXP \circ H)w = -e^T(P^TXP \circ H)^{-1}(P^TXP \circ H)w \\ &= -e^Tw < 0. \end{aligned}$$

Since H is extremal for $\mathcal{C}_5^*$ (cf. [7]) and $w > 0$, it follows that $\mathrm{Diag}(w)H\mathrm{Diag}(w)$ is extremal for $\mathcal{C}_5^*$, and consequently K is extremal for $\mathcal{C}_5^*$. Therefore, some $\widehat{Y} \in \mathcal{C}_5$ with $K \bullet \widehat{Y} = 0$ must exist. This proves the last statement of the theorem. □

Note that by Corollary 2 we know that any $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ can be written in the form

$$X = Y + Z, \quad Y \in \mathcal{C}_5, \quad Z \in \mathcal{E}_5. \tag{21}$$

Theorem 8 provides a mechanism for separating X from $\mathcal{C}_5$ when $Y = 0$ in (21). In fact when X has the form (21) where $Y \neq 0$, it may not be possible to "separate" X from $\mathcal{C}_5$ because X itself could be CP. This possibility was demonstrated in the example at the end of Section 3. The question of how to separate an arbitrary $X \in \mathcal{D}_5 \setminus \mathcal{C}_5$ from $\mathcal{C}_5$ is an interesting open problem and is closely related to the problem of finding a full outer description of $\mathcal{C}_5$.

As an application of Theorem 8 we consider the problem of computing the maximum stable set in a graph. Let A be the adjacency matrix of a graph G on n vertices, and let α be the maximum size of a stable set in G. It is known [6] that

$$\alpha^{-1} = \min\left\{(I + A) \bullet X : ee^T \bullet X = 1, X \in \mathcal{C}_n\right\}. \tag{22}$$

Relaxing $\mathcal{C}_n$ to $\mathcal{D}_n$ results in a polynomial-time computable upper bound on α:

$$(\vartheta')^{-1} = \min\left\{(I + A) \bullet X : ee^T \bullet X = 1, X \in \mathcal{D}_n\right\}. \tag{23}$$

The bound ϑ' was first established (via a different derivation) by Schrijver as a strengthening of the Lovász ϑ number.

Because the feasible set of (22) is simply the set of normalized CP matrices, the extreme points of (22) are simply the normalized rank-1 CP matrices. Similarly these normalized rank-1 CP matrices together with the normalized extremely bad matrices constitute the extreme points of (23). For $n = 5$, this fact and the results of Section 4 give rise to the following uniqueness result for (23).

Proposition 1. *If* $n = 5$ *and* $\alpha < \vartheta'$, *then* (23) *has a unique optimal solution* $X^* \in \mathcal{E}_5$.

Proof. We prove the contrapositive. Suppose that there exist two optimal solutions X_1 and X_2 such that $X_1 \neq X_2$. Then $X_3 := (X_1 + X_2)/2$ is optimal and also CP-reducible because it is not extreme in $\mathcal{D}_5$. Hence, there exists $0 \neq Y \in \mathcal{C}_5$ and $Z \in \mathcal{D}_5$, both with unit component-wise sum, and $\gamma \in (0, 1)$ such that $X_3 = \gamma Y + (1 - \gamma)Z$. Because X_3 is optimal and both Y and Z are feasible, it follows that Y is optimal. However, since Y is also feasible for (22), this shows $\vartheta' = \alpha$. $\square$

We now investigate implications of Proposition 1 and Theorem 8 for the canonical 5-cycle C, for which

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}. \tag{24}$$

In this case, $\alpha = 2$ and $\vartheta' = \sqrt{5} > 2$ (see [6]). Letting $\bar{A} = ee^T - (I + A)$ denote the adjacency matrix of the complement 5-cycle, it is straightforward to verify that

$$X^* = \left(\frac{1}{5\sqrt{5}}\right) I + \left(\frac{\sqrt{5} - 1}{10\sqrt{5}}\right) \bar{A}$$

is the unique optimal solution of (23) with $(I + A) \bullet X^* = 1/\sqrt{5}$.

Next, we derive the cut which separates X^* from $\mathcal{C}_5$ in accordance with Theorem 8. The permutation matrix P that obtains $G(P^T X^* P) = C$ corresponds to the permutation vector $\pi = (1, 4, 2, 5, 3)$, resulting in

$$P^T X^* P = \left(\frac{1}{5\sqrt{5}}\right) I + \left(\frac{\sqrt{5} - 1}{10\sqrt{5}}\right) A.$$

We next compute $w = -(P^T X^* P \circ H)^{-1} e \approx 47.3607e$. Since w is a positive multiple of e we can simply rescale and take $w = e$. Then $K = P \mathrm{Diag}(w) H \mathrm{Diag}(w) P^T = PHP^T$, and the desired cut is $K \bullet X = H \bullet P^T X P \geqslant 0$. Adding this cut to (23) results in the optimization problem

$$\min \left\{ (I + A) \bullet X : ee^T \bullet X = 1, X \in \mathcal{D}_5, K \bullet X \geqslant 0 \right\}, \tag{25}$$

which has optimal value 1/2. For example, the rank-1 CP matrix $(e_1 + e_3)(e_1 + e_3)^T$ is easily verified to be an optimal solution. In other words, for the case of A given in (24), the single cut derived above is sufficient to close the gap between (23) and (22).

Previous papers have considered other strengthenings of (23) that are sufficient to close the gap between (23) and (22) for the case of A from (24). In [6] this is accomplished by using a better approximation of the dual cone $\mathcal{D}_5^*$, and the proof that the improved dual problem attains the objective value 1/2 makes use of the Horn matrix (7). The approach taken in [4] is similar to (25) in that a single linear inequality is added to (23). In fact, simple manipulations using the relationship $\bar{A} = ee^T - (I + A)$, the form of H, and the constraint $ee^T \bullet X = 1$ show that the cut $K \bullet X \geqslant 0$ generated above is equivalent to the constraint $(I + A) \bullet X \geqslant 1/2$, which is the inequality added in [4]. However, the derivation of this additional constraint in [4] appears to be unrelated to our derivation via Theorem 8.

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