On the number of CP factorizations of a completely positive matrix

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ABSTRACT
A square matrix $A$ is completely positive if $A = BB^T$, where $B$ is a (not necessarily square) nonnegative matrix. In general, a completely positive matrix may have many, even infinitely many, such CP factorizations. But in some cases a unique CP factorization exists. We prove a simple necessary and sufficient condition for a completely positive matrix whose graph is triangle free to have a unique CP factorization. This implies uniqueness of the CP factorization for some other matrices on the boundary of the cone $CP_n$ of $n \times n$ completely positive matrices. We also describe the minimal face of $CP_n$ containing a completely positive $A$. If $A$ has a unique CP factorization, this face is polyhedral.

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1. Introduction

An $n \times n$ matrix $A$ is said to be completely positive if $A = BB^T$ for some (entrywise) nonnegative $B$. The matrix $B$ need not be square, and typically the completely positive $A$ has many, often infinitely many, such factorizations. The minimal number of columns in such a nonnegative factor $B$ is called the cp-rank of $A$, and denoted by $cpr A$. A factorization $A = BB^T, B \geq 0$, is called a CP factorization of $A$, and if $B$ has $cpr A$ columns, a minimal CP factorization. These are also, in general, not unique. In this paper we consider the number of CP factorizations and minimal CP factorizations of a given completely positive matrix.

Determining whether a given matrix is completely positive is hard (in complexity terms, NP-hard – see [1]). Finding the cp-rank of a known completely positive matrix is also hard: one CP factorization does not lead naturally to all others, or to a minimal one. These difficult problems have gained an increased interest in the last couple of decades, due to the use of completely positive matrices in optimization. The $n \times n$ completely positive matrices form a convex cone $CP_n$ in the space $S_n$ of $n \times n$ symmetric matrices. The dual of this cone is the cone $COP_n$ of $n \times n$ copositive matrices. (An $n \times n$ matrix $A$ is copositive if $x^T Ax \geq 0$ for every nonnegative vector $x \in \mathbb{R}^n$.) It has been shown that a wide family of difficult optimization problems, both discrete and continuous, may be reformulated as
linear optimization problems with a matrix variable in either $\mathcal{CP}_n$ or $\mathcal{COP}_n$. In such a formulation, the difficulty of the problem is shifted to the cone. Hence the increased interest in the matrices in the cones $\mathcal{CP}_n$ and $\mathcal{COP}_n$, and also in the structure of these cones. For details on copositive optimization see [2, 3]. See [4] for a survey on complete positivity. An updated and extended book by the same authors, titled *Copositive and Completely Positive Matrices*, is due to appear soon, containing, as the name suggests, also an up-to-date survey on copositivity. See [5] for open problems in this field. Although some work has been done on these problems since the paper appeared, they are still generally open.

The number of CP factorizations has not been widely explored so far, but some results do exist. The number of minimal CP factorizations was considered in [6] for completely positive matrices whose graph is a cycle, in [7] for matrices that have an acyclic or a unicyclic graph, and in [8] for certain positive matrices on the boundary of $\mathcal{CP}_5$. In [9] completely positive matrices with a chordal graph and minimal possible rank were shown to have a unique CP factorization. Even fewer papers deal with the structure of $\mathcal{CP}_n$. Some geometry results may be found in [10], and faces of $\mathcal{CP}_5$ were studied in [11, 12]. (The latter two papers contain also examples of matrices in $\mathcal{CP}_5$ that have unique CP factorizations.)

The main result in this paper is a simple necessary and sufficient condition for a completely positive matrix whose graph is triangle free to have a unique CP factorization. This result generalizes both the results of [6, 7] in two ways: we consider the wider family of matrices with triangle free graphs, and consider also CP factorizations that are not minimal. We will also show that this result may be applied to find the number of CP factorizations of additional matrices on the boundary of $\mathcal{CP}_n$ (some of them positive), in particular those considered in [8]. We conclude with a description of the minimal face of $\mathcal{CP}_n$ containing a completely positive $A$ – both in the general case and in the special case that $A$ has a unique CP representation, demonstrating the implication of this uniqueness.

The paper is organized as follows: In the next section we establish mainly notation and terminology. In Section 3 we make some initial observations and state some results regarding the number of CP factorizations of a completely positive matrix. In Section 4 we state and prove the main result about matrices with triangle free graphs, and demonstrate its relevance to other matrices on the boundary. In Section 5 we describe the minimal face of $\mathcal{CP}_n$ containing a completely positive $A$ in the general case, and in the case that $A$ has a unique CP representation.

### 2. Notation and terminology

Vectors are denoted by lower bold case letters, with the $i$th entry of a vector $x$ denoted by $x_i$. Matrices are denoted by capital letters. In particular, $e_1, \ldots, e_n$ are the standard basis vectors in $\mathbb{R}^n$, $0$ is the zero vector, and $e$ is the vector of all ones. The $n \times n$ zero matrix is $0_n$, and $E_{ij}$ is a square matrix all of whose entries are zero, except for 1 in the $i, j$ position. For a vector $x \in \mathbb{R}^n$, $\text{supp } x = \{ 1 \leq i \leq n \mid x_i \neq 0 \}$ is the support of $x$. We say that $x$ is a nonnegative (positive) vector, and write $x \geq 0$ ($x > 0$), if all its entries are nonnegative (positive); $\mathbb{R}_+^n = \{ x \mid x \geq 0 \}$ is the nonnegative orthant of $\mathbb{R}^n$. Similarly, we write $A \geq 0$ ($A > 0$) and say that $A$ is nonnegative (positive) if all the entries of the matrix $A$ are nonnegative (positive). A diagonal matrix is called positive if all its diagonal elements are positive. A signature matrix is a diagonal matrix with 1 and -1 entries on the diagonal. If $\sigma \subseteq \{ 1, \ldots, n \}$, we denote by $x[\sigma]$ the restriction of the vector $x \in \mathbb{R}^n$ to the indices in $\sigma$. 
and by \( A[\sigma] \) the principal submatrix of an \( n \times n \) matrix \( A \) whose rows and columns are indexed by \( \sigma \). We denote by \( A(\sigma) \) the principal submatrix of \( A \) on the rows and columns indexed by the complement of \( \sigma \), \( A(\sigma \mid \sigma) \) is the submatrix whose rows are indexed by \( \sigma \), and its columns by the complement of \( \sigma \), and \( A(\sigma \mid \sigma) \) is submatrix whose rows are indexed by the complement of \( \sigma \), and its rows by the complement of \( \sigma \). If \( A[\sigma] \) is nonsingular, the Schur complement of \( A[\sigma] \) in \( A \) is defined as

\[
A/A[\sigma] = A(\sigma) - A(\sigma \mid \sigma)A[\sigma]^{-1}A(\sigma \mid \sigma).
\]

An \( M \)-matrix is a square matrix of the form \( dI - Q \), where \( Q \) is a nonnegative matrix, and \( d \geq \rho(Q) \), the spectral radius of \( Q \). The comparison matrix of a square matrix \( A \), \( M(A) \), is defined by

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

Some details on these matrix notions may be found in [4, Chapter 1]. A good general reference on matrix theory is [13], and [14] is a recommended reference for \( M \)-matrices, their many equivalent definitions and their properties. For our purposes it is important that a symmetric matrix with nonnegative diagonal elements and nonpositive off-diagonal elements is an \( M \)-matrix if and only if it is positive semidefinite, and that an irreducible symmetric \( M \)-matrix has a positive eigenvector corresponding to its smallest eigenvalue, which is simple. This implies that a symmetric \( M \)-matrix \( S \) is positive semidefinite if and only if for some positive diagonal \( D \) the matrix \( DSD \) is diagonally dominant. Note also that \( M(A) \) is diagonally dominant if and only if \( A \) is diagonally dominant, and recall that an irreducible diagonally dominant matrix is nonsingular if and only if in at least one row the diagonal dominance is strict. Regarding the Schur complement one should keep in mind that if \( A \) is positive semidefinite and \( A[\sigma] \) is nonsingular, then \( A/A[\sigma] \) is a positive semidefinite matrix and \( \text{rank} A/A[\sigma] = \text{rank} A - \text{rank} A[\sigma] \).

We use basic graph theoretic notions, which may be found in standard textbooks on graph theory, see, e.g. [15]. We only consider graphs that are simple (undirected, no loops, no multiple edges). We denote by \( cc(G) \) the (edge-)clique covering number of a graph \( G \), the minimal number of cliques needed to cover \( G \)'s edges. A graph is triangle free if the largest cliques in the graph are its edges, hence for a triangle free graph \( cc(G) \) is the number of edges in \( G \). The graph of a symmetric \( n \times n \) matrix \( A \), denoted by \( G(A) \), has vertex set \( \{1, \ldots, n\} \) and \( \{i,j\} \) is an edge if and only if \( a_{ij} \neq 0 \). The matrix \( A \) is irreducible if and only if \( G(A) \) is connected.

We will recall known results on completely positive matrices and the cones \( \mathcal{C}P_n \) and \( \mathcal{COP}_n \) as we go along. When no explicit reference is given, references can be found in [4]. For now, we only mention this: An obvious necessary condition for \( A \) to be completely positive is that it is doubly nonnegative, i.e. both positive semidefinite and entrywise nonnegative. However, this necessary condition is not sufficient. A graph \( G \) is called completely positive if every doubly nonnegative matrix with this graph is completely positive. Completely positive graphs were fully characterized: these are exactly the graphs that contain no odd cycle on five vertices or more. In particular, all bipartite graphs are completely positive.
3. Initial results on the number of CP factorizations

We first point out that the CP factorization \( A = BB^T, B \geq 0 \), is equivalent to

\[
A = \sum_{i=1}^{k} b_i b_i^T, \quad b_i \geq 0, \quad i = 1, \ldots, k,
\]

where \( b_1, \ldots, b_k \) are the columns of \( B \). We refer to this sum as a CP representation, and if the CP factorization is minimal, as a minimal CP representation. We use CP factorizations and CP representations interchangeably. To avoid artificially extended CP factorizations, we only consider CP factorizations \( A = BB^T \) where in the nonnegative \( B \) no column is a scalar multiple of another (that is, the columns of \( B \) are pairwise linearly independent). Two CP factorizations \( A = BB^T \) and \( A = CC^T \) are considered equal if \( C \) and \( B \) only differ by the order of their columns (that is, \( C = BP \) for some permutation matrix \( P \)).

If \( A = A_1 \oplus A_2 \oplus \cdots \oplus A_m \), then the number of CP factorizations of \( A \) is completely determined by the number of CP factorizations of the direct summands. The matrix \( A \) has infinitely many CP factorizations if and only if at least for one \( i \) the matrix \( A_i \) has infinitely many CP factorizations. If \( A_i \) has \( k_i \) different CP factorizations, then \( A \) has \( \prod_{i=1}^{m} k_i \) different CP factorizations. We may therefore simplify the discussion by restricting our attention to irreducible matrices.

As usual when considering completely positive matrices, we rely on the fact that if \( A \) is a symmetric matrix, \( P \) is a permutation matrix and \( D \) is a positive diagonal matrix, all of the same order, then \( A \) is completely positive matrix if and only if \( PAP^T \) is, if and only if \( DAD \) is. For our purposes it is also important to note that

\[
A = BB^T \iff DAD = (DB)(DB)^T, \\
A = BB^T \iff PAP^T = (PB)(PB)^T.
\]

Since such \( P \) and \( D \) have nonnegative inverses, these equivalences imply a one-to-one correspondence between CP factorizations of \( A \) and those of \( DAD \), or \( PAP^T \). We may therefore apply diagonal scaling and permutation similarity to our matrices without changing the number of (minimal) CP factorizations.

With these basic observations in mind, we state some initial results regarding the number of CP factorizations.

An obvious example of a completely positive matrix with a unique CP factorization is any rank 1 matrix \( bb^T, b \in \mathbb{R}_+^n \). For matrices of rank 2, we recall an idea that dates back to [16], and reestablished since then in many papers, including [7], in several variations. Since this is a basis for several more observations, we include a proof. Recall that the cp-rank satisfies \( \text{cpr} A \geq \text{rank} A \), and may be much larger than the rank. However, equality holds if \( \text{rank} A = 1 \) or \( \text{rank} A = 2 \).

**Observation 3.1:** Let \( b_1, b_2 \in \mathbb{R}_+^n \) be linearly independent, and have \( \text{supp} b_1 \supseteq \text{supp} b_2 \). Then \( A = b_1 b_1^T + b_2 b_2^T \) has infinitely many minimal CP factorizations.

**Proof:** Let \( B = [b_1 \ b_2] \). Each of the \( n \) rows of \( B \) is in the nonnegative quadrant of \( \mathbb{R}^2 \), and has a positive first entry. Hence no two rows are orthogonal to each other, and there
are infinitely many possible rotations that keep these \( n \) vectors \( \mathbb{R}^2 \), hence infinitely many orthogonal \( 2 \times 2 \) matrices \( R \) such that \( BR \geq 0 \), with different \( R \)'s resulting in different \( BR \)'s.

Note that if \( A = BB^T, B \geq 0 \), is a CP factorization, then the support of each column of \( B \) is a clique in \( G(A) \), and these cliques cover all the edges of \( G(A) \). Hence \( cpr A \geq cc (G) \).

In [9, Theorem 1 and Corollary 1] it was shown that if \( A \) is a completely positive matrix with a chordal graph (a graph that has no induced cycle greater than a triangle), and \( \text{rank} A = cc (G(A)) \), then \( A \) has a unique CP representation. Combining this result with Observation 3.1, we get the following corollary.

**Corollary 3.1:** An irreducible rank \( 2 \) completely positive matrix \( A \) has a unique CP representation if and only if \( A \) has a zero off-diagonal entry in a row and column that are nonzero. If \( A \) does not have such a zero off-diagonal entry, then it has infinitely many minimal CP representations.

**Proof:** Since \( cpr A = \text{rank} A = 2 \), we have that \( cc (G(A)) \leq 2 \). The matrix \( A \) has a zero off-diagonal entry in a row and column that are nonzero if and only if \( cc (G(A)) \geq 2 \) (since \( A \) is irreducible, each row/column has at least one positive off-diagonal entry). Hence we need to show that if \( cc (G(A)) = 2 \), \( A \) has a unique CP representation, and if \( cc (G(A)) = 1 \), \( A \) has infinitely many CP representations. The first claim follows from [9, Theorem 1 and Corollary 1].

If \( cc (G(A)) = 1 \), in any minimal CP representation \( A = b_1 b_1^T + b_2 b_2^T \) the support of one of the vectors includes the support of the other. (Otherwise there exist \( i \in \text{supp} b_2 \setminus \text{supp} b_1 \), and \( j \in \text{supp} b_1 \setminus \text{supp} b_2 \), and then \( a_{ij} = 0 \) and \( cc (G(A)) \geq 2 \).) By Observation 3.1 such a CP representation yields infinitely many others. 

The interior of \( \mathcal{CP}_n \) was described in [17], and the description was refined in [18]. The interior consists of nonsingular matrices \( A \) that have a CP factorization \( A = BB^T \) in which at least one column of \( B \) is positive. From Observation 3.1 we therefore get the following.

**Corollary 3.2:** Any matrix in the interior of \( \mathcal{CP}_n, n \geq 2 \), has infinitely many CP factorizations.

**Proof:** Let \( A = BB^T \) be a CP factorization of \( A \) with a positive column. Without loss of generality, \( b_1 > 0 \). By Observation 3.1, we may replace columns \( b_1 \) and \( b_2 \) by infinitely many other pairs of columns, to obtain infinitely many CP factorizations of \( A \).

However, in [19] it was shown that there are matrices in the interior of \( \mathcal{CP}_n \) that do not have a minimal CP factorization with a positive column. We do not know the answer to the following question:

**Question 3.1:** Does there exist a matrix \( A \) in the interior of \( \mathcal{CP}_n \) which has a unique minimal CP factorization, or finitely many such factorizations?

The main result of this paper generalizes the result of [6], where it was shown that a completely positive matrix \( A \) whose graph is a cycle has a unique minimal CP representation if \( M(A) \) is singular, and two if \( M(A) \) is nonsingular. The proof there is by determinant
computations. The result also generalizes the results of [7], where the possible values of the number of minimal CP representations were found in the case that the graph of the matrix is either a tree or unicyclic. The proofs there are by an algorithm that computes a minimal CP factorization, and reveals the number of possible outcomes. Since the proof of the main theorem relies on the result for trees, we provide here for completeness a direct proof. It uses the same principles as the ones used in the algorithm of [7], and in the proof for general chordal graphs in [9], in particular, the known fact that an $n \times n$ completely positive matrix whose graph is a tree has rank at least $n-1$ and cp-rank equal to the rank.

**Theorem 3.3 ([7]):** Let $A$ be an $n \times n$ completely positive matrix whose graph is a tree, $n \geq 2$. If $A$ is singular, then $A$ has a unique minimal CP factorization. If $A$ is nonsingular, then $A$ has infinitely many CP factorizations.

**Proof:** We prove the result for singular matrices by induction on $n$. For $n = 2$, this is simply the fact that a rank 1 completely positive matrix has a unique CP representation. Suppose the result holds for $n - 1 \geq 2$, and let $A$ by an $n \times n$ singular completely positive matrix whose graph is a tree. Then $\text{cpr} \ A = \text{rank}A = n - 1$, and each minimal CP representation has $n-1$ columns, each supported by an edge of $G(A)$. Without loss of generality we may assume that 1 is a pendant vertex in $G(A)$, adjacent only to 2. Then

$$A = \begin{bmatrix}
  a_{11} & a_{12} & 0 & \cdots & 0 \\
  a_{12} & 0 & \cdots & \cdots & \cdots \\
  \vdots & \vdots & \ddots & \ddots & \ddots \\
  0 & 0 & \cdots & 0 & A(1)
\end{bmatrix}.$$ 

In any minimal CP representation of $A$, exactly one of the vectors, say $b_1$, is supported by $\{1, 2\}$. Necessarily

$$b_1b_1^T = \begin{bmatrix}
  a_{11} & a_{12} \\
  a_{12} & a_{11}
\end{bmatrix} \oplus 0_{n-2}.$$ 

Hence

$$A - b_1b_1^T = 0_1 \oplus A/A[1]$$

is doubly nonnegative, and its rank is one less than rank$A$, i.e. $n-2$. The graph of $A/A[1]$ is the tree obtained from $G(A)$ by deleting the vertex 1 and the edge incident with it. As trees are completely positive graphs, $A/A[1]$ is a completely positive singular matrix, and by the induction hypothesis this matrix has a unique minimal CP representation as a sum of $n-2$ rank 1 matrices. Hence $A - b_1b_1^T$ has a unique minimal CP representation

$$A - b_1b_1^T = \sum_{i=2}^{n} b_ib_i^T,$$

and $A = \sum_{i=1}^{n} b_ib_i^T$ is the only minimal CP representation of $A$. 
If $A$ is an $n \times n$ nonsingular matrix whose graph is a tree, then $\text{cpr} \ A = n$. It has a minimal CP representation

$$A = \sum_{i=1}^{n} b_i b_i^T.$$ 

In this CP representation, $n-1$ of the vectors $b_1, \ldots, b_n$ have to be supported by the $n-1$ different edges of $G(A)$. The support of the $n$th vector is contained in the support of one of these $n-1$ vectors. Without loss of generality, we may assume $\text{supp} \ b_2 \subseteq \text{supp} \ b_1$. By Observation 3.1, one may obtain infinitely many different CP representation by replacing $b_1 b_1^T + b_2 b_2^T$. ■

Our main result generalizes also the results of [6, 7] regarding the number of CP factorizations of completely positive matrices whose graph is a cycle or unicyclic, except that it does not give an indication on the maximum number of minimal CP factorizations of a unicyclic graph. For completeness, we state and prove here this part. The proof is different from the original proofs, but like them relies on the fact that a completely positive matrix whose graph is triangle free and not a tree has cp-rank equal to the number of edges of the graph.

**Theorem 3.4 ([6, 7]):** Let $A$ be an $n \times n$ irreducible completely positive matrix whose graph contains exactly one cycle, on $k \geq 4$ vertices. Then $A$ has at most two minimal CP factorizations.

**Proof:** First suppose $G(A)$ is a cycle. By considering an appropriate permutation similarity, we assume that

$$A = \begin{bmatrix}
d_1 & h_1 & 0 & \ldots & 0 & h_n \\
h_1 & d_2 & h_2 & \ddots & \vdots & 0 \\
0 & h_2 & d_3 & h_3 & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & h_{n-2} & d_{n-1} & h_{n-1} \\
h_n & 0 & \ldots & 0 & h_{n-1} & d_n
\end{bmatrix},$$

where $h_i$ and $d_i$ are positive, $i = 1, \ldots, n$. Each minimal CP representation of $A$ consists of $n$ summands $b_i b_i^T$, with each $b_i$ supported by one of the $n$ edges of the graph. Without loss of generality,

$$b_1 b_1^T = \begin{bmatrix} t & h_1 \\
h_1 & h_1^2 / t \end{bmatrix} \oplus 0_{n-2}, \quad t > 0.$$
Then

\[
A - b_1 b_1^T = \begin{bmatrix}
d_1 - t & 0 & 0 & \ldots & 0 & h_n \\
0 & d_2 - \frac{h_1^2}{t} & h_2 & \ddots & 0 \\
0 & h_2 & d_3 & h_3 & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & 0 \\
0 & \ldots & h_{n-2} & d_{n-1} & h_{n-1} & h_n \\
h_n & 0 & \ldots & 0 & h_{n-1} & d_n
\end{bmatrix}
\]

is a completely positive matrix which has a CP representation with \(n-1\) summands, and its graph is a path on \(n\) vertices. In particular,

\[
\text{rank}(A - b_1 b_1^T) = \text{cpr}(A - b_1 b_1^T) = n - 1.
\]

By the previous result, \(A - b_1 b_1^T\) has a unique CP representation. Hence the number of CP representations of \(A\) is equal to the number of positive \(t\)’s for which \(A - b_1 b_1^T\) is doubly nonnegative and singular. The last \(n-2\) columns in the positive semidefinite \(A' = A - b_1 b_1^T\) are linearly independent by their sign pattern, hence the principal submatrix \(A'(1, 2) = A(1, 2)\) is nonsingular. As \(\text{rank} A' = n - 1\), the matrix \(A'/A(1, 2)\) is positive semidefinite and has rank 1. This latter matrix has the form

\[
A'/A(1, 2) = \begin{bmatrix}
a - t & b \\
b & c - \frac{h_1^2}{t}
\end{bmatrix},
\]

for some real numbers \(a, b, c\). Hence \(\det(A'/A(1, 2)) = 0\) translates into a quadratic equation in \(t\), that has at most two positive solutions.

The result for a unicyclic graph may be deduced by induction on \(n-k\), by removing at the induction step one vector from the minimal CP representation, supported by a pendant edge, as in the previous proof.

\[\square\]

4. Completely positive matrices with a triangle free graph

In this section we prove our main result. We begin with some background material to put it in context. In [20] a simple non-combinatorial sufficient condition for complete positivity was proved: If \(A\) is a symmetric nonnegative matrix whose comparison matrix \(M(A)\) is positive semidefinite, then \(A\) is completely positive. In the case that the graph of \(A\) is triangle free, this sufficient condition is also necessary. In [21] a simple alternative proof for this latter theorem was suggested. We describe it here, since this idea will be used in the next proof. If \(G(A)\) is triangle free, then the support of every column in a CP factorization of \(A\) is contained in one of the edges of \(G(A)\). For a nonnegative vector \(b\) with \(|\text{supp } b| = 2\), we have \(M(bb^T) = dd^T\), where \(d\) is obtained from \(b\) by reversing the sign of exactly one nonzero element in \(b\). Therefore if \(A = \sum_{i=1}^k b_i b_i^T\), where for each \(i\) the support of \(b_i\) is of size at most 2, we have \(M(A) = \sum_{i=1}^k d_i d_i^T\), where \(d_i d_i^T = M(b_i b_i^T)\) is a rank one positive semidefinite matrix, with \(\text{supp } d_i = \text{supp } b_i\), \(|d_i| = b_i\). (If \(|\text{supp } b_i| = 1\) simply take \(d_i = b_i\).) Hence \(M(A)\) is positive semidefinite.
Our main result concerns exactly these completely positive matrices with triangle free graph.

**Theorem 4.1:** Let $A$ be an $n \times n$ irreducible completely positive matrix, $n \geq 2$, whose graph is triangle free. Then the following are equivalent

(a) $M(A)$ is singular.  
(b) $A$ has a unique CP factorization.  
(c) $A$ has a unique minimal CP factorization.

**Remark 4.2:** If the triangle free $G(A)$ is bipartite, then $A$ is singular if and only if $M(A)$ is singular: Let $\alpha_1$ and $\alpha_2$ be the independent sets of vertices in $G(A)$ such that every edge has one end in $\alpha_1$ and the other in $\alpha_2$. Then $A = SM(A)S$, where $S$ is the signature matrix with

$$s_{ii} = \begin{cases} 1, & i \in \alpha_1 \\ -1, & i \in \alpha_2 \end{cases}.$$  

In particular, in the case that $G(A)$ is a tree, (a) $\implies$ (c) of Theorem 4.1 is the first part of Theorem 3.3.

Also, if $G(A)$ is bipartite and $A$ is a nonsingular, then for every $i$ there exists $\delta > 0$ such that $A - \delta E_{ii}$ is a singular completely positive matrix. To see that, assume for convenience that $i = n$. Then

$$\det(A - \delta E_{nn}) = \det A - \delta \det A(n).$$

As $A(n)$ is nonsingular we get that for $\delta = \det A / \det A(n)$ the matrix $A' = A - \delta E_{nn}$ is singular. It is positive semidefinite, since it has a nested sequence of $n$ leading principal minors, all positive except for the determinant of the matrix itself, which is zero. Hence also the $n$th diagonal element of $A'$ is nonnegative, and $A'$ is a doubly nonnegative matrix, and its graph is $G(A)$.

Both observations in Remark 4.2 will be used in the proof of Theorem 4.1.

**Proof of Theorem 4.1:** Only (a) $\implies$ (b) and (c) $\implies$ (a) need to be proved.

(a) $\implies$ (b): Let $A = \sum_{i=1}^{k} b_i b_i^T$ be any CP representation of $A$. The support of each $b_i$ is contained in an edge of $G(A)$, hence $1 \leq |\text{supp } b_i| \leq 2$ for every $i$. Then, as explained above,

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

where $M(b_i b_i^T) = d_i d_i^T$ is a rank one positive semidefinite matrix, with $\text{supp } d_i = \text{supp } b_i$, $|d_i| = b_i$.

The irreducible $M$-matrix $M(A)$ is singular, hence it has a positive eigenvector $v$ corresponding to the eigenvalue zero. Then from $M(A) = \sum_{i=1}^{k} d_i d_i^T$, we get that each $d_i$ is in the column space of $M(A)$, and is therefore orthogonal to $v$. Since $1 \leq |\text{supp } d_i| \leq 2$, this forces $\sigma_i = \text{supp } d_i$ to have size 2, and hence $d_i[\sigma_i]$ spans the orthogonal complement $\{v[\sigma_i]\}^\perp$ in $\mathbb{R}^2$. As the vectors $b_1, \ldots, b_k$ are pairwise linearly independent, so are
\( \mathbf{d}_1, \ldots, \mathbf{d}_k \). Combined with the fact that \( \{ \mathbf{v}[\sigma_i]\}^\perp \) is one dimensional, this implies that \( \text{supp} \mathbf{d}_j \neq \sigma_i \) for every \( j \neq i \). Therefore if \( \sigma_i = \{p, q\} \), we have \( (\mathbf{d}_i \mathbf{d}_i^T)_{pq} = (M(A))_{pq} \). This equality, together with \( \mathbf{d}_i^T \mathbf{v} = 0 \), completely determines \( \mathbf{d}_i \) up to sign, and hence also determines \( \mathbf{b}_i = |\mathbf{d}_i| \). This shows that the representation \( A = \sum_{i=1}^{k} \mathbf{b}_i \mathbf{b}_i^T \) is unique (and necessarily \( k = |E(G(A))| \)).

(c) \( \Rightarrow \) (a): We will show that if \( M(A) \) is nonsingular, then \( A \) has at least two minimal CP factorizations. As the number of CP factorizations is preserved by positive diagonal congruence, it suffices to prove the following claim: If \( M(A) \) is diagonally dominant and nonsingular, then \( A \) has at least two different minimal CP representations. We prove the claim by induction on the number \( m \) of edges of the connected \( G(A) \). Recall that the number of summands in a minimal CP representation of such \( A \) is \( m \).

Consider first the case that \( G(A) \) is a tree, \( m = n-1 \). As \( M(A) \) is a nonsingular diagonally dominant matrix, \( A \) is also nonsingular by Remark 4.2. Since \( G(A) \) is a tree, \( \text{cpr} \ A = \text{rank} A \), and any minimal CP representation of \( A \) has \( n \) summands. We can generate two different minimal CP representations as follows. Choose \( \delta_1 > 0 \) such that \( A - \delta_1 E_{11} \) is positive semidefinite and singular, and \( \delta_2 > 0 \) such that \( A - \delta_2 E_{22} \) is positive semidefinite and singular (\( \delta_i = \text{det}(A)/\text{det}(A(\sigma_i)), i = 1, 2 \)). Both matrices are doubly nonnegative, with the same tree graph as \( A \), and are therefore completely positive. By Remark 4.2, both their comparison matrices are also singular. As (a) implies (b), there exist unique CP representations

\[
A - \delta_1 E_{11} = \sum_{i=1}^{n-1} \mathbf{b}_i \mathbf{b}_i^T \quad \text{and} \quad A - \delta_2 E_{22} = \sum_{i=1}^{n-1} \mathbf{c}_i \mathbf{c}_i^T,
\]

where for each \( i \) the nonnegative vectors \( \mathbf{b}_i \) and \( \mathbf{c}_i \) are supported by the same edge of the tree. Then

\[
A = \delta_1 E_{11} + \sum_{i=1}^{n-1} \mathbf{b}_i \mathbf{b}_i^T \quad \text{and} \quad A = \delta_2 E_{22} + \sum_{i=1}^{n-1} \mathbf{c}_i \mathbf{c}_i^T
\]

are two minimal rank 1 representations of \( A \) that are clearly different (by the only vector in each representation that is supported by a single vertex).

Now suppose the claim holds for \( m \geq n - 1 \), and let \( A \) be an irreducible completely positive matrix with a nonsingular diagonally dominant comparison matrix, whose triangle free graph \( G(A) \) has \( m + 1 \) edges. As \( M(A) \) is nonsingular, there exists \( 1 \leq i \leq n \) such that in row \( i \) there is strict diagonal dominance, i.e. \( (M(A)\mathbf{e})_i > 0 \). As \( G(A) \) is not a tree, there exists an edge whose removal from \( G(A) \) will keep the graph connected. Without loss of generality \( \{1, 2\} \) is such an edge. Let \( F = \begin{bmatrix} a_{12} & -a_{12} \\ a_{12} & a_{12} \end{bmatrix} \oplus 0_{n-2} \). Since \( F\mathbf{e} = 0 \), we have \( (M(A) - F)\mathbf{e} = M(A)\mathbf{e} \geq 0 \) and

\[
((M(A) - F)\mathbf{e})_i = (M(A)\mathbf{e})_i > 0.
\]

Hence \( M(A) - F = M(A - |F|) \) is a nonsingular diagonally dominant matrix whose graph has \( m \) edges. By the induction hypothesis, \( A - |F| \) has at least two different minimal CP
representations,

\[ A - |F| = \sum_{i=1}^{m-1} b_i b_i^T \quad \text{and} \quad A - |F| = \sum_{i=1}^{m-1} c_i c_i^T. \]

Then

\[ A = |F| + \sum_{i=1}^{m-1} b_i b_i^T \quad \text{and} \quad A = |F| + \sum_{i=1}^{m-1} c_i c_i^T \]

are two different minimal CP representations of \( A \).

In the case that \( G(A) \) is a tree, \( A \) has infinitely many minimal CP factorizations by Theorem 3.3. The following corollary extends this to a bipartite \( G(A) \).

**Corollary 4.3:** Let \( A \) be an \( n \times n \) irreducible completely positive matrix, whose graph is bipartite. Then

(a) If \( A \) is singular, it has a unique CP factorization. 
(b) If \( A \) is nonsingular, it has at least two minimal CP factorizations, and infinitely many CP factorizations.

**Proof:** By Remark 4.2, in this case \( M(A) \) is singular if and only if \( A \) is. Therefore (a), and the first part of (b), follow from Theorem 4.1.

If \( A \) is nonsingular, we may choose \( \delta > 0 \) such that \( A' = A - \delta E_{11} \) is singular and positive semidefinite. Then \( A' \) is doubly nonnegative with \( G(A') = G(A) \) bipartite, and therefore \( A' \) is completely positive and singular. By part (a), \( A' \) has a unique CP representation

\[ A' = \sum_{i=1}^{m} b_i b_i^T, \]

where each \( b_i \) is supported by an edge in \( G(A') \). Without loss of generality, \( 1 \in \text{supp } b_1 \). Then

\[ A = \delta E_{11} + b_1 b_1^T + \sum_{i=2}^{k} b_i b_i^T. \]

As \( \delta E_{11} + b_1 b_1^T = (\sqrt{\delta} e_1)(\sqrt{\delta} e_1)^T + b_1 b_1^T \), and \( \text{supp } \sqrt{\delta} e_1 \subseteq \text{supp } b_1 \), the result follows from Observation 3.1.

In the case that \( G(A) \) is an \( n \)-cycle, \( n \geq 4 \), by Theorem 3.4 the completely positive matrix \( A \) has either one or two minimal CP factorizations. Theorem 4.1 gives us an easy way to determine how many minimal CP factorizations \( A \) has. In the next corollary we state the result in terms of a given CP factorization of the cyclic \( A \).
Corollary 4.4: Let \( A \) be a completely positive matrix whose graph is the \( n \)-cycle \( 1 - 2 - \cdots - n - 1 \). Then the CP factorization \( A = BB^T \), where

\[
B = \begin{bmatrix}
  s_1 & 0 & 0 & \ldots & t_n \\
  t_1 & s_2 & 0 & \ldots \\
  0 & t_2 & \ddots & \ddots \\
  \vdots & \vdots & \ddots & 0 \\
  0 & 0 & \ldots & s_{n-1} & 0 \\
  0 & 0 & 0 & \ldots & t_{n-1} & s_n
\end{bmatrix}, \quad s_i, t_i > 0, \ i = 1, \ldots, 5, \tag{1}
\]

is the unique CP factorization of \( A \) if and only if \( \prod_{i=1}^n s_i = \prod_{i=1}^n t_i \).

Proof: We have \( M(A) = S S^T \), where \( S \) is obtained from \( B \) by replacing each \( t_i \) by \(-t_i\). Therefore \( \det M(A) = (\prod_{i=1}^n s_i - \prod_{i=1}^n t_i)^2 \) (whether \( n \) is even or odd!), and \( M(A) \) is singular if and only if \( \prod_{i=1}^n s_i = \prod_{i=1}^n t_i \). \( \blacksquare \)

Although Theorem 4.1 holds for matrices whose graph is triangle free, in some cases it has implications on the number of (minimal) CP factorizations of other completely positive matrices that lie on the boundary of the cone \( \mathcal{CP}_n \). Getting into that requires a brief reminder regarding \( \mathcal{CP}_n \), its dual \( \mathcal{COP}_n \) and the matrices on their boundaries. The inner product in \( S_n \) is \( \langle A, B \rangle = \text{trace}(AB) \). The mutual duality of the cones \( \mathcal{CP}_n \) and \( \mathcal{COP}_n \) is with respect to this inner product:

\[
\mathcal{CP}_n^* = \{ X \in S_n \mid \langle X, Y \rangle \geq 0 \ \text{for every} \ Y \in \mathcal{CP}_n \} = \mathcal{COP}_n,
\]

and

\[
\mathcal{COP}_n^* = \{ X \in S_n \mid \langle X, Y \rangle \geq 0 \ \text{for every} \ Y \in \mathcal{COP}_n \} = \mathcal{CP}_n.
\]

In particular, matrices on the boundary of \( \mathcal{CP}_n \) are orthogonal to matrices on the boundary of \( \mathcal{COP}_n \). So if \( M \) is on the boundary of \( \mathcal{COP}_n \), there exists a nonzero nonnegative vector \( b \) such that

\[
b^T M b = \langle M, bb^T \rangle = 0.
\]

Such \( b \) is called a zero of \( M \), and if \( \text{supp} \ b \) does not strictly contain a support of another zero, \( b \) is called a minimal zero of \( M \). In [22] it was proved that each copositive \( M \) has a finite number of minimal zeros, up to multiplication by a scalar, and every zero of \( M \) is a nonnegative combination of a finite number of minimal zeros. We call a set of minimal zeros of \( M \) representative if every minimal zero of \( M \) is a scalar multiple of exactly one vector in the set. Symmetric nonnegative matrices are copositive, and so are the positive semidefinite matrices. For \( n \geq 5 \) there exist copositive matrices in \( \mathcal{COP}_n \) that are not a sum of a positive semidefinite matrix and a symmetric nonnegative one. Such a copositive matrix is called exceptional. From [22] we know that if an exceptional matrix in \( \mathcal{COP}_n \) generates an extreme ray of the cone (i.e. it is extremal), then it has at least \( n \) representative minimal zeros that span \( \mathbb{R}^n \).

Lemma 4.5: Let \( M \) be an \( n \times n \) exceptional extremal copositive matrix, that has exactly \( n \) representative minimal zeros, \( w_1, \ldots, w_n \). Let \( W = [w_1 \ w_2 \ \ldots \ w_n] \). Then each completely
positive matrix $A$, which is orthogonal to $M$ in $S_n$, has the form $A = WCW^T$ for some $n \times n$ completely positive $C$, $\text{cpr } A = \text{cpr } C$, and and the number of (minimal) CP factorizations of $A$ is equal to the number of (minimal) CP factorizations of $C$.

**Proof:** By the assumptions on $M$, the nonnegative matrix $W$ is nonsingular. Each zero of $M$ is a nonnegative combination of $W$’s columns. If $A = BB^T$ for some nonnegative $B$, each column of $B$ is a zero of $M$, hence $B = WX$, where $X \geq 0$, and

$$A = (WX)(WX)^T = WCW^T,$$

where $C = XX^T$ is a completely positive matrix. By (2), $\text{cpr } A \leq \text{cpr } C$.

If $A = QQ^T$ is any CP factorization of $A$, then $Q = WY$, $Y \geq 0$. Since

$$A = QQ^T = W(YY^T)W^T$$

and $W$ is nonsingular, we get that $YY^T = W^{-1}AW^{-T} = C$ is a CP factorization of $C$. In particular, if $A = QQ^T$ is a minimal CP factorization, this shows that $\text{cpr } C \leq \text{cpr } A$, and we conclude that $\text{cpr } A = \text{cpr } C$. As $W$ is nonsingular, $B \neq Q$ if and only if $X \neq Y$. Hence the number of CP factorizations/minimal CP factorizations of both matrices are equal. ■

Given a completely positive matrix orthogonal to an exceptional extremal copositive matrix, which has $n$ representative minimal zeros, we may compute $C = W^{-1}AW^{-T}$. If the matrix $C$ has a triangle free graph, it is easy to check by its comparison matrix whether it has a unique CP factorization. However, for general $n$ finding the exceptional extremal matrices in $\text{COP}_n$ is a major open problem. These were characterized fully only for $n = 5$ in [23] and for $n = 6$ in [24]. But some examples of exceptional extremal matrices are known for every $n$.

In $\text{COP}_5$ one exceptional extremal matrix is the Horn matrix

$$H = \begin{bmatrix}
1 & -1 & 1 & 1 & -1 \\
-1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
1 & 1 & -1 & 1 & -1 \\
-1 & 1 & 1 & -1 & 1
\end{bmatrix}.$$  

Other exceptional extremal matrices in $\text{COP}_5$ are the matrices called Hildebrand matrices. We do not describe these here, but mention that each Hildebrand matrix has exactly five zeros, up to scalar multiplication; all these zeros are minimal, and each has support of size 3. Every exceptional extremal matrix in $\text{COP}_5$ is obtained from either the Horn matrix or from a Hildebrand matrix by permutation similarity and diagonal scaling.

We can demonstrate the use of the Lemma 4.5 in conjunction with Theorem 4.1 for some $5 \times 5$ matrices.
Example 4.6: The minimal zeros of the Horn matrix $H$ are

$$w_i = e_i + e_{i+1}, \quad i = 1, \ldots, 5,$$

where $+$ denotes addition modulo 5 on $\{1, \ldots, 5\}$. Let

$$W = [w_1 \ w_2 \ w_3 \ w_4 \ w_5] = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$ 

The matrix

$$A = \begin{bmatrix} 8 & 5 & 1 & 1 & 5 \\ 5 & 8 & 5 & 1 & 1 \\ 1 & 5 & 8 & 5 & 1 \\ 1 & 1 & 5 & 8 & 5 \\ 5 & 1 & 1 & 5 & 8 \end{bmatrix}$$

is an example of a completely positive matrix orthogonal to $H$ (introduced in [17]). The matrix

$$C = W^{-1}AW^{-T} = \begin{bmatrix} 3 & 1 & 0 & 0 & 1 \\ 1 & 3 & 1 & 0 & 0 \\ 0 & 1 & 3 & 1 & 0 \\ 0 & 0 & 1 & 3 & 1 \\ 1 & 0 & 0 & 1 & 3 \end{bmatrix}$$

has a cyclic graph and a strictly diagonally dominant comparison matrix, hence $C$, and therefore $A$, has two minimal CP factorizations. Moreover, $C$, and therefore $A$, has infinitely many CP factorizations. For example, for every $0 < t < 1$ the matrix $C - tI$ has two minimal CP factorizations. Let $C - tI = U(t)U(t)^T$ be a minimal CP factorization of $C - tI$ (one of the two). Then

$$C = [\sqrt{t}I_5 \ U(t)][\sqrt{t}I_5 \ U(t)]^T, \quad 0 < t < 1$$

are infinitely many different CP factorizations of $C$, and $A = V(t)V(t)^T$, where

$$V(t) = W[\sqrt{t}I_5 \ U(t)],$$

are infinitely many CP factorizations of $A$ (not all).

On the other hand,

$$A' = \begin{bmatrix} 6 & 4 & 1 & 1 & 4 \\ 4 & 6 & 4 & 1 & 1 \\ 1 & 4 & 6 & 4 & 1 \\ 1 & 1 & 4 & 6 & 4 \\ 4 & 1 & 1 & 4 & 6 \end{bmatrix}$$
has a unique CP representation:

\[
C' = W^{-1}A'W^{-T} = \begin{bmatrix}
2 & 1 & 0 & 0 & 1 \\
1 & 2 & 1 & 0 & 0 \\
0 & 1 & 2 & 1 & 0 \\
0 & 0 & 1 & 2 & 1 \\
1 & 0 & 0 & 1 & 2
\end{bmatrix}
\]

has a singular comparison matrix. The unique CP factorization of \(C'\) happens to be

\[
C' = WW^T,
\]

and the unique CP factorization of \(A'\) is therefore \(A' = W^2(W^2)^T\), where

\[
W^2 = \begin{bmatrix}
1 & 0 & 0 & 1 & 2 \\
2 & 1 & 0 & 0 & 1 \\
1 & 2 & 1 & 0 & 0 \\
0 & 1 & 2 & 1 & 0 \\
0 & 0 & 1 & 2 & 1
\end{bmatrix}.
\]

We mention that it was already shown in [8, Theorems 4.1 and 4.4] that any positive completely positive matrix \(A\) orthogonal to the Horn matrix has \(\text{cpr} A = \text{rank} A\), and at most two minimal CP factorization, but without the simple rule to determine the exact number. If \(A\) is positive, then \(A = (WB)(WB)^T\), where \(B\) is as in (1). In this case \(\text{cpr} A = \text{rank} A = \text{rank} B = 5\). Lemma 4.5 combined with Corollary 4.4 yield a characterization, previously obtained in [12], of when is a given minimal CP factorization of such \(A\) unique.

Now consider matrices in \(CP_5\) there are orthogonal to a Hildebrand matrix. mentioned above a Hildebrand matrix has exactly five minimal zeros, all minimal, up to scalar multiplication, any completely positive matrix orthogonal to a Hildebrand matrix has a unique factorization \(A = VDV^T\), where \(V\) is the matrix of representative zeros of the Hildebrand matrix, and \(D\) is a nonnegative diagonal matrix. As such \(D\) has a unique CP factorization (as a direct sum of rank 1 matrices...), so does \(A\). This was previously proved (for a positive \(A\)) in [8, Theorem 4.4].

These examples are not unique to \(CP_5\). Matrices in \(CP_n, n \geq 6\), that are orthogonal to certain exceptional extremal matrices in \(COP_n\) have unique CP factorizations. Results from [25] show that exceptional extremal ‘Hildebrand-like’ matrices exist in \(COP_n\) for every odd order \(n \geq 5\) (with \(n\) representative zeros, all minimal, whose supports are the sets \(\{1, \ldots, n\} \setminus \{i, i+1\}\), where + denotes addition modulo \(n\) on \(\{1, \ldots, n\}\)). Completely positive matrices orthogonal to these matrices have a unique CP factorization. By [25], exceptional extremal ‘Horn-like’ matrices exist in \(COP_n\) for every \(n \geq 5\) (with zeros whose supports are the sets \(\{1, \ldots, n\} \setminus \{i, i+1\}\), where + denotes addition modulo \(n\) on \(\{1, \ldots, n\}\), each of which is a sum of two minimal zeros). Specific examples of such exceptional extremal matrices were constructed for every \(n \geq 5\) in [25, Section 7]. Completely positive matrices orthogonal to these matrices have either one or two minimal CP factorizations, similarly to completely positive matrices that are orthogonal to the Horn matrix.
5. The minimal face of $\mathcal{CP}_n$ containing $A$

The facial structure of the completely positive cone is of interest, and not yet thoroughly explored. We recall that a subcone $\mathcal{F}$ of a convex cone $\mathcal{K}$ is a face of $\mathcal{K}$ if $X, Y \in \mathcal{K}$ and $X + Y \in \mathcal{F}$ implies that both $X$ and $Y$ are in $\mathcal{F}$. In this section we demonstrate the implication of the existence of a unique CP factorization regarding the minimal face of $\mathcal{CP}_n$ containing a given completely positive matrix $A$. Let us denote the minimal face of $\mathcal{CP}_n$ containing $A$ by $\mathcal{F}_{\mathcal{CP}_n}^A$. It is a face of $\mathcal{CP}_n$ that contains $A$ and is contained in every face that contains $A$ (it is the intersection of all such faces). For an arbitrary completely positive matrix $A$ on the boundary of $\mathcal{CP}_n$, the description of $\mathcal{F}_{\mathcal{CP}_n}^A$ is as follows.

**Theorem 5.1:** Let $A \in \mathcal{CP}_n$. Then the minimal face of $\mathcal{CP}_n$ containing $A$ is

$$\mathcal{F}_{\mathcal{CP}_n}^A = \text{cone}\{bb^T \mid b \in \mathbb{R}_+^n \text{ and } A - bb^T \in \mathcal{CP}_n\}$$

**Proof:** Let us denote $\mathcal{K} = \text{cone}\{bb^T \mid b \in \mathbb{R}_+^n \text{ and } A - bb^T \in \mathcal{CP}_n\}$. To show that $\mathcal{K}$ is the minimal face containing $A$, we will show that it is a face, and any face containing $A$ contains the whole $\mathcal{K}$. We start with the latter. Let $\mathcal{F}$ be a face of $\mathcal{CP}_n$ containing $A$, and let $b$ be any nonnegative vector such that $A - bb^T$ is completely positive, then

$$A = bb^T + (A - bb^T) \in \mathcal{F}$$

implies that $bb^T \in \mathcal{F}$. Hence $\{bb^T \mid b \in \mathbb{R}_+^n \text{ and } A - bb^T \in \mathcal{CP}_n\} \subseteq \mathcal{F}$, and since $\mathcal{F}$ is a cone, $\mathcal{K} \subseteq \mathcal{F}$.

Now we show that $\mathcal{K}$ is a face of $\mathcal{CP}_n$. First, if $A = B + C$, $B, C \in \mathcal{CP}_n$, and $B = \sum_{i=1}^k b_i b_i^T$ is a CP representation of $B$, then for each $1 \leq i \leq k$ the matrix

$$A - b_j b_j^T = \sum_{1 \leq j \leq k \atop j \neq i} b_j b_j^T + C$$

is completely positive. Hence each $b_i \in \mathcal{K}$, and therefore $B = \sum_{i=1}^k b_i b_i^T \in \mathcal{K}$. Similarly $C \in \mathcal{K}$.

Now suppose $X$ is any matrix in $\mathcal{K}$. Then $X = \sum_{i=1}^m t_i v_i v_i^T$, where $v_i \in \mathbb{R}_+^n$, $t_i > 0$ and $A - v_i v_i^T \in \mathcal{CP}_n$ for every $i$. Let $t = \sum_{i=1}^k t_i$. If $X = Y + Z$, where $Y, Z \in \mathcal{CP}_n$, write

$$A = \frac{1}{t} Y + \frac{1}{t} \left( Z + \sum_{i=1}^m t_i (A - v_i v_i^T) \right).$$

Then $\frac{1}{t} Y \in \mathcal{K}$, and reversing the roles of $Y$ and $Z$, also $\frac{1}{t} Z \in \mathcal{K}$. Hence $\mathcal{K}$ is a face. ■

Note that checking whether $bb^T$ is in this face requires checking complete positivity of a matrix, hence it is not an easy task. In the common case that $A$ has infinitely many CP factorizations, $\mathcal{F}_{\mathcal{CP}_n}^A$ has infinitely many extreme rays. In the special case that $A$ has a unique CP representation, the description of $\mathcal{F}_{\mathcal{CP}_n}^A$ is more tangible, and $\mathcal{F}_{\mathcal{CP}_n}^A$ is a polyhedral cone.
**Corollary 5.2:** Let $A \in \mathcal{CP}_n$ have a unique CP representation $A = \sum_{i=1}^{k} b_i b_i^T$. Then the minimal face of $\mathcal{CP}_n$ containing $A$ is

$$F^A_{\mathcal{CP}_n} = \text{cone}\{b_i b_i^T \mid 1 \leq i \leq k\}.$$

**Proof:** For a nonnegative vector $b \in \mathbb{R}^n$, $bb^T$ may be completed to a CP representation of $A$ if and only if $b$ is one of $b_1, \ldots, b_k$. ■

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**References**

[1] Dickinson PJC, Gijben L. On the computational complexity of membership problems for the completely positive cone and its dual. Comput Optim Appl. 2014;57(2):403–415.

[2] Dür M. Copositive programming: a survey. In: Diehl M, Glineur F, Jarlebring E, Michiels W, editors. Recent advances in optimization and its applications in engineering. Berlin: Springer; 2010. p. 3–20.

[3] Bomze IM. Copositive optimization – recent developments and applications. Eur J Oper Res. 2012;216(3):509–520.

[4] Berman A, Shaked-Monderer N. Completely positive matrices. River Edge (NJ): World Scientific; 2003.

[5] Berman A, Dür M, Shaked-Monderer N. Open problems in the theory of completely positive and copositive matrices. Electron J Linear Algebra. 2015;29:46–58.

[6] Zhang X-D, Li J-S. Completely positive matrices having cyclic graphs. J Math Res Expo. 2000;20(1):27–31.

[7] Dickinson PJC, Dür M. Linear-time complete positivity detection and decomposition of sparse matrices. SIAM J Matrix Anal Appl. 2012;33(3):701–720.

[8] Shaked-Monderer N, Bomze IM, Jarre F, Schachinger W. On the cp-rank and minimal cp factorizations of a completely positive matrix. SIAM J Matrix Anal Appl. 2013;34(2):355–368.

[9] Shaked-Monderer N. Matrices attaining the minimum semidefinite rank of a chordal graph. Linear Algebra Appl. 2013;438(10):3804–3816.

[10] Dickinson PJC. Geometry of the copositive and completely positive cones. J Math Anal Appl. 2011;380(1):377–395.

[11] Zhang Q. Completely positive cones: are they facially exposed. Linear Algebra Appl. 2018;558:195–204.

[12] Zhang Q. Faces of the $5 \times 5$ completely positive cone. Linear Multilinear Algebra. 2020;68(12):2523–2540.

[13] Horn RA, Johnson CR. Matrix analysis. 2nd ed. Cambridge: Cambridge University Press; 2013.

[14] Berman A, Plemmons RJ. Nonnegative matrices in the mathematical sciences. Philadelphia (PA): Society for Industrial and Applied Mathematics (SIAM); 1994. (Classics in applied mathematics; vol. 9). Revised reprint of the 1979 original.

[15] Diestel R. Graph theory. 5th ed. Berlin: Springer; 2018. (Graduate texts in mathematics; vol. 173).

[16] Hall M. Combinatorial theory. 2nd ed. New York: Wiley; 1998. (Wiley classics library).

[17] Dür M, Still G. Interior points of the completely positive cone. Electron J Linear Algebra. 2008;17:48–53.

[18] Dickinson PJC. An improved characterisation of the interior of the completely positive cone. Electron J Linear Algebra. 2010;20:723–729.

[19] Bomze IM, Dickinson PJC, Still G. The structure of completely positive matrices according to their CP-rank and CP-plus-rank. Linear Algebra Appl. 2015;482:191–206.
[20] Drew JH, Johnson CR, Loewy R. Completely positive matrices associated with $M$-matrices. Linear Multilinear Algebra. 1994;37(4):303–310.
[21] Berman A, Shaked-Monderer N. Remarks on completely positive matrices. Linear Multilinear Algebra. 1998;44(2):149–163.
[22] Hildebrand R. Minimal zeros of copositive matrices. Linear Algebra Appl. 2014;459:154–174.
[23] Hildebrand R. The extreme rays of the $5 \times 5$ copositive cone. Linear Algebra Appl. 2012;437(7):1538–1547.
[24] Afonin A, Dickinson PJC, Hildebrand R. The extreme rays of the $6 \times 6$ copositive cone. J Glob Optim. In press.
[25] Hildebrand R. Copositive matrices with circulant zero support set. Linear Algebra Appl. 2017;514:1–46.