A SEMIDEFINITE RELAXATION ALGORITHM FOR CHECKING COMPLETELY POSITIVE SEPARABLE MATRICES

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Abstract. A symmetric matrix $A$ is completely positive (CP) if there exists an entrywise nonnegative matrix $V$ such that $A = VV^T$. A real symmetric matrix is called completely positive separable (CPS) if it can be written as a sum of rank-1 Kronecker products of completely positive matrices. This paper studies the CPS problem. A criterion is given to determine whether a given matrix is CPS, and a specific CPS decomposition is constructed if the matrix is CPS.

1. Introduction. Let $n$ be a positive integer. Denote by $S_n$ the space of $n \times n$ real symmetric matrices. For $A \in S_n$, $A \succeq 0$ (resp., $A \geq 0$) means that $A$ is a symmetric entrywise nonnegative (resp., positive semidefinite) matrix. A symmetric matrix $A \in S_n$ is completely positive (CP) if there exist nonnegative vectors $v_1, \ldots, v_r \in \mathbb{R}_n^+$ such that

$$A = v_1v_1^T + \cdots + v_rv_r^T. \tag{1}$$

The number $r$ is called the length of the decomposition (1) and the smallest length of (1) is called the CP-rank of $A$. If $A$ is CP, we call (1) a CP-decomposition of $A$. So, $A$ is CP if and only if $A = VV^T$ for an entrywise nonnegative matrix $V$.

Clearly, a CP matrix is doubly nonnegative (DNN), i.e., it is not only positive semidefinite but also nonnegative entrywise. Denote

$$\mathcal{CP}_n = \{A \in S_n : A = VV^T \text{ with } V \succeq 0\},$$

$$\mathcal{DNN}_n = \{B \in S_n : B \succeq 0, B \geq 0\},$$

the completely positive cone, and the doubly nonnegative cone, respectively. It was shown in [2] that $\mathcal{CP}_n = \mathcal{DNN}_n$ holds only for $n \leq 4$. The cone $\mathcal{CP}_n$ is a proper cone (i.e., closed, convex, pointed and full-dimensional). It is also well-known that checking the membership in $\mathcal{CP}_n$ is NP-hard, while checking the membership in its dual cone is co-NP-hard [8, 19].

Completely positive matrices have wide applications in combinatorics and statistics. For example, the block designs, maximin efficiency-robust tests and Markovian

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model of DNA evolution need to check the complete positivity of a given matrix [2]. A lot of problems in applications can be formulated as completely positive programming problem. Interested readers are referred to [1, 3, 9, 33].

Let $p$ and $q$ be two positive integers. For matrices $B \in S_p$ and $C \in S_q$, $B \otimes C$ denotes their Kronecker product, i.e., $B \otimes C$ is the block matrix

$$B \otimes C := (B_{ik}C_{jk})_{1 \leq i,k \leq p}.$$ 

Let $K_{p,q}$ be the subspace spanned by all such Kronecker products:

$$K_{p,q} = \text{span}\{B \otimes C : B \in S_p, C \in S_q\}.$$ 

The set $K_{p,q}$ is a proper subspace of $S_{pq}$, and its dimension is

$$\dim K_{p,q} = \frac{1}{4}p(p+1)q(q+1).$$

If both $B \in S_p$ and $C \in S_q$ are rank-1, we call $B \otimes C$ a rank-1 Kronecker product. A matrix is called separable if it can be written as a nonnegative linear combination of rank-1 Kronecker product of semidefinite matrices. Checking whether or not a density matrix is separable is important in quantum information theory [5]. A quantum system is separable (resp., entangled) if its density matrix is separable (resp., not separable). We refer to [7, 11, 24] for recent work on entanglement or separability.

Given two positive integers $p$ and $q$, a matrix $A \in K_{p,q}$ is said to be completely positive separable (CPS) if there exists $B_j \in CP_p, C_j \in CP_q (j = 1, 2, \ldots, r)$ such that

$$A = B_1 \otimes C_1 + \cdots + B_r \otimes C_r,$$ 

where $pq = n, 1 < p, q < n$. The equation (3) is called a CPS-decomposition of $A$. Denote by $CP_{p,q}$ the cone of all such completely positive separable matrices:

$$CP_{p,q} = \left\{ \sum_{j=1}^r B_j \otimes C_j : \text{each } B_j \in CP_p, C_j \in CP_q, r \in \mathbb{N} \right\}.$$ 

The completely positive separable matrices have lots of applications in biquadratic polynomial optimization (see Section 6).

In this paper, we study how to determine whether a given symmetric matrix is CPS or not. We show that the CPS problem is equivalent to a truncated moment problem with special structures, then construct a hierarchy of semidefinite relaxations for solving it. If a matrix is not CPS, we can give a certificate for that. If it is, we can give a CPS-decomposition for it.

The paper is organized as follows. In Section 2, we present some preliminaries in the field of polynomial optimization and truncated moment problems. In Section 3, we reformulate the problem of checking CPS matrices as a truncated moment problem and study the properties of the CPS cone. A semidefinite relaxation algorithm is proposed to check whether a matrix is CPS or not in Section 4, and the convergence of the algorithm is also analysed. Some computational results are given in Section 5. Finally, we summarize the paper and discuss the applications of CPS matrices in biquadratic polynomial optimization in Section 6.
2. Preliminaries. Notation. The symbol \( \mathbb{N} \) (resp., \( \mathbb{R} \)) denotes the set of nonnegative integral (resp., real) numbers. For \( t \in \mathbb{R} \), \( \lfloor t \rfloor \) denotes the smallest integer that is greater than or equal to \( t \). Denote \( [t] := \{1, \ldots, n\} \). Let \( p, q \) be positive integers. Given variables \( x \in \mathbb{R}^p, y \in \mathbb{R}^q \), denote \( (x, y) = (x_1, \ldots, x_p, y_1, \ldots, y_q) \in \mathbb{R}^p \times \mathbb{R}^q \).

Let \( \mathbb{R}[x, y] := \mathbb{R}[x_1, \ldots, x_p, y_1, \ldots, y_q] \) be the ring of polynomials in \((x, y)\) with real coefficients and \( \mathbb{M}[x, y] \subseteq \mathbb{R}[x, y] \) be the set of all real monomials in \((x, y)\). For a monomial \( \Omega \subseteq \mathbb{M}[x, y] \) and a pair \((a, b) \in \mathbb{R}^p \times \mathbb{R}^q\), \( [(a, b)]_{\Omega} \) denotes the vector of all monomials in \( \Omega \) evaluated at the point \((a, b)\). For \( d > 0 \), \( \mathbb{M}[x, y] \) (resp., \( \mathbb{R}[x, y] \)) denotes the set of all monomials (resp., polynomials) with degrees at most \( d \). When \( \Omega = \mathbb{M}[x, y] \), the vector \( [(a, b)]_{\mathbb{M}[x, y]} \) is denoted by \( [(a, b)]_{d} \). For a set \( S \subseteq \mathbb{N}^n \), \(|S|\) denotes its cardinality, and \( \text{int}(S) \) denotes its interior. Clearly, the dimension of the vector \( [(a, b)]_{d} \) is \( |\mathbb{M}[x, y]| = (\dim^{+}d)^d \). For \( v \in \mathbb{R}^n \), denote \( \|v\|_2 := \sqrt{v^T v} \). In the following, we introduce some concepts, terminology and notations in polynomial optimization, which are inherited from [14].

2.1. Polynomial optimization. An ideal \( I \) in \( \mathbb{R}[x, y] \) is a subset of \( \mathbb{R}[x, y] \) such that \( I \cdot \mathbb{R}[x, y] \subseteq I \) and \( I + I \subseteq I \). For a tuple \( h = (h_1, \ldots, h_s) \) in \( \mathbb{R}[x, y] \), denote by \( I(h) \) the ideal generated by \( h \), which is the set

\[
I(h) = h_1 \cdot \mathbb{R}[x, y] + \cdots + h_s \cdot \mathbb{R}[x, y].
\]

We also denote the \( k \)-th truncation of the ideal \( I(h) \) as

\[
I_k(h) := h_1 \cdot \mathbb{R}[x, y]_{k-{\deg}(h_1)} + \cdots + h_s \cdot \mathbb{R}[x, y]_{k-{\deg}(h_s)}. \tag{5}
\]

Clearly, \( I(h) = \bigcup_{k \in \mathbb{N}} I_k(h) \).

A polynomial \( f \in \mathbb{R}[x, y] \) is called a sum of squares (SOS) if there exist \( f_1, \ldots, f_l \in \mathbb{R}[x, y] \) for some \( l \in \mathbb{N} \) such that \( f = f_1^2 + \cdots + f_l^2 \). The set of all SOS polynomials in \((x, y)\) is denoted by \( \Sigma[x, y] \). For a degree \( d \), denote the truncation

\[
\Sigma[x, y]_d := \Sigma[x, y] \cap \mathbb{R}[x, y]_d.
\]

It is a closed convex cone for all even \( d > 0 \). For a tuple \( g := (g_1, \ldots, g_i) \) of polynomials in \( \mathbb{R}[x, y] \), the quadratic module generated by \( g \) is the set

\[
Q(g) := \Sigma[x, y] + g_1 \cdot \Sigma[x, y] + \cdots + g_i \cdot \Sigma[x, y]. \tag{6}
\]

The \( 2k \)-th truncation of \( Q(g) \) is the set

\[
Q_{2k}(g) := \Sigma[x, y]_{2k} + g_1 \cdot \Sigma[x, y]_{d_1} + \cdots + g_i \cdot \Sigma[x, y]_{d_i}, \tag{7}
\]

where each \( d_i = 2k - \deg(g_i) \). Then, \( Q(g) = \bigcup_{k \in \mathbb{N}} Q_{2k}(g) \).

Let \( h \) and \( g \) be the polynomial tuples as above. Denote

\[
S(h, g) = \{(x, y) \in \mathbb{R}^p \times \mathbb{R}^q : h(x, y) = 0, g(x, y) \geq 0\}. \tag{8}
\]

It is clear that if \( f \in I(h) + Q(g) \), then \( f \geq 0 \) on \( S(h, g) \). In fact, the converse is also true under some general conditions. When \( I(h) + Q(g) \) is archimedean (i.e., there exists \( N \) such that \( N - \|x\|^2 - \|y\|^2 \in I(h) + Q(g) \)), if \( f > 0 \) on \( S(h, g) \), then \( f \in I(h) + Q(g) \). This is called Putinar’s Positivstellensatz in the literature (cf. [25]). Moreover, as shown recently in [23], if \( f \geq 0 \) on \( S(h, g) \), then we also have \( f \in I(h) + Q(g) \) under some general optimality conditions. We refer to [16, 17] for more details in polynomial optimization.
2.2. Localizing matrices and flat extension. For \( \alpha = (\alpha_1, \ldots, \alpha_p) \in \mathbb{N}^p \) and \( \beta = (\beta_1, \ldots, \beta_q) \in \mathbb{N}^q \), denote monomial \( x^\alpha y^\beta := x_1^{\alpha_1} \cdots x_p^{\alpha_p} y_1^{\beta_1} \cdots y_q^{\beta_q} \) and
\[
|\alpha| := \alpha_1 + \ldots + \alpha_p, \quad |\beta| := \beta_1 + \ldots + \beta_q.
\]
Let \( \mathbb{R}^{[x,y]_d} \) be the space of real vectors indexed by monomials in the set \( M[x,y]_d \), i.e., for a vector \( w \in \mathbb{R}^{[x,y]_d} \), we index it as
\[
w = (w_{x^\alpha y^\beta})_{x^\alpha y^\beta \in M[x,y]_d}.
\]
For example, let \( p = 1, q = 2, d = 2 \), \( x \in \mathbb{R}^p, y = (y_1, y_2) \in \mathbb{R}^q \), then
\[
M[x,y]_d = \{1, x, y_1, y_2, x^2, xy_1, xy_2, y_1^2, y_2^2\}.
\]
A vector \( w = (1, 2, \ldots, 10)^T \in \mathbb{R}^{[x,y]_d} \) implies that its elements is indexed as
\[
w_1 = 1, w_x = 2, \ldots, w_{y_2}^2 = 10.
\]
We call such vector \( w \in \mathbb{R}^{[x,y]_d} \) a truncated multi-sequence (tms) of degree \( d \).

For a polynomial \( f \in \mathbb{R}[x,y]_d \) and a tms \( w \in \mathbb{R}^{[x,y]_d} \), define the scalar product
\[
\langle f, \alpha, \beta \rangle := \sum_{|\alpha|+|\beta| \leq d} f_{x^\alpha y^\beta} w_{x^\alpha y^\beta},
\]
where \( f_{x^\alpha y^\beta} \) are the coefficients of the polynomial \( f \in \mathbb{R}[x,y]_d \). We say that the tms \( w \) admits an \( S(h,g) \)-representing measure if there exists a nonnegative Borel measure \( \mu \) such that its support is contained in \( S(h,g) \) and
\[
w_{x^\alpha y^\beta} = \int x^\alpha y^\beta d\mu, \quad \forall x^\alpha y^\beta \in M[x,y]_d.
\]
If so, such \( \mu \) is called an \( S(h,g) \)-representing measure for \( w \).

For a polynomial \( f \in \mathbb{R}[x,y]_{2k} \), the \( k \)-th localizing matrix of \( f \) generated by \( w \in \mathbb{R}^{[x,y]_{2k}} \) is the symmetric matrix \( L_f^{(k)}(w) \) satisfying
\[
\langle f \phi_1 \phi_2, w \rangle = \text{vec}(\phi_1)^T (L_f^{(k)}(w)) \text{vec}(\phi_2), \quad \forall \phi_1, \phi_2 \in \mathbb{R}[x]_{k-\lceil \text{deg}(f)/2 \rceil}.
\]
In the above, \( \text{vec}(\phi) \) denotes the coefficient vector of the polynomial \( \phi \) in the graded lexicographical ordering. In particular, when \( f = 1 \) (the constant one polynomial), \( L_f^{(1)}(w) \) is called a moment matrix and is denoted as
\[
M_k(w) := L_f^{(1)}(w).
\]
The columns and rows of \( L_f^{(k)}(w) \), as well as \( M_k(w) \), are indexed by monomials \( x^\alpha y^\beta \in \mathbb{M}[x,y]_{k-\lceil \text{deg}(f)/2 \rceil} \).

Recall that \( h = (h_1, \ldots, h_s) \) and \( g = (g_1, \ldots, g_t) \) are two polynomial tuples. For convenience, denote
\[
\begin{align*}
L_h^{(k)}(w) &:= \text{diag} \left\{ L_{h_1}^{(k)}(w), \ldots, L_{h_s}^{(k)}(w) \right\}, \\
L_g^{(k)}(w) &:= \text{diag} \left\{ L_{g_1}^{(k)}(w), \ldots, L_{g_t}^{(k)}(w) \right\}.
\end{align*}
\]
In the above, \( \text{diag}(X_1, \ldots, X_r) \) denotes the block diagonal matrix whose diagonal blocks are \( X_1, \ldots, X_r \). Let \( S(h,g) \) be given as in (8). In applications, an interesting question is how to check whether or not a tms \( w \in \mathbb{R}^{[x,y]_{2k}} \) admits an \( S(h,g) \)-representing measure. For this to be true, a necessary condition (cf. [4, 21]) is that
\[
L_h^{(k)}(w) = 0, \quad L_g^{(k)}(w) \succeq 0, \quad M_k(w) \succeq 0.
\]
However, the converse is typically not true. Let \( d_0 = \max\{1, \lceil \deg(h)/2 \rceil, \lceil \deg(g)/2 \rceil \} \). If \( w \) satisfies (13) and the rank condition
\[
\operatorname{rank} M_{k-d_0}(w) = \operatorname{rank} M_k(w),
\]
then \( w \) admits a unique \( S(h,g) \)-representing measure \( \mu \), which is supported on \( r := \operatorname{rank} M_k(w) \) distinct points in \( S(h,g) \) (cf. Curto and Fialkow [4]). We say that \( w \) is flat with respect to \( h \) and \( g \), if (13) and (14) are both satisfied.

For two tms’ \( w \in \mathbb{R}^{M[x,y]/2k} \) and \( z \in \mathbb{R}^{M[x,y]/2l} \) with \( k < l \), we say that \( z \) is an extension of \( w \), if \( w_x^a y^b = z_x^a y^b \) for all \( x^a y^b \in M[x,y]/2k \). For convenience, we denote by \( z|_{d} \) the subvector of \( z \) whose entries are indexed by \( x^a y^b \in M[x,y]/d \). If \( z|_{2k} = w \) and \( z \) is flat, we say that \( z \) is a flat extension of \( w \). Flat extensions are very useful for checking whether a tms \( w \) admits an \( S(h,g) \)-representing measure or not.

3. Reformulation and properties of completely positive separable matrices. In this section, we formulate the problem of checking completely positive separable matrices as a special truncated moment problem. The properties of the cone of completely positive separable matrices are also discussed.

3.1. Reformulation. Recall the matrix space \( K_{p,q} \) as in (2). Denote
\[
E = \{(i,j,k,l): 1 \leq i \leq k \leq p, 1 \leq j \leq l \leq q\}.
\]
Then the dimension of the space \( K_{p,q} \) is the cardinality \( |E| = \frac{1}{2}p(p+1)q(q+1) \).

Thus, each \( A \in K_{p,q} \) can be identified by the vector
\[
a \in \mathbb{R}^E
\]
such that \( a_{ijkl} = A(i-1)q+j, (k-1)q+l \) for all \((i,j,k,l) \in E\). Such a vector \( a \in \mathbb{R}^E \) is called the identifying vector of \( A \in K_{p,q} \).

By the definition, each completely positive separable matrix in \( CP_{p,q} \) is a non-negative linear combination of rank-1 Kronecker products like \((aa^T) \otimes (bb^T)\), where \( a^T a = b^T b = 1 \), \( a \in \mathbb{R}^p \), \( b \in \mathbb{R}^q \). Denote the set
\[
\Delta := \{(x,y) \in \mathbb{R}^p \times \mathbb{R}^q : x^T x = 1, y^T y = 1, x \geq 0, y \geq 0 \}.
\]
Thus, \( A \in CP_{p,q} \) if and only if
\[
A = \sum_{s=1}^{r} \rho_s (a_s a_s^T) \otimes (b_s b_s^T)
\]
for \( \rho_1, \ldots, \rho_r > 0 \) and \((a_1, b_1), \ldots, (a_r, b_r) \in \Delta\). Furthermore, the above is also equivalent to its identifying vector \( a \) satisfying
\[
a_{ijkl} = \sum_{s=1}^{r} \rho_s (a_s)_i (b_s)_j (a_s)_k (b_s)_l, \quad \forall (i,j,k,l) \in E.
\]
If we denote
\[
\mathcal{E} = \{x_i y_j x_k y_l : 1 \leq i \leq k \leq p, 1 \leq j \leq l \leq q\},
\]
then the monomial \( x_i y_j x_k y_l \in \mathcal{E} \) can be uniquely identified by the tuple \((i,j,k,l) \in E \) as in (15). Since there is a one-to-one correspondence between \( E \) and \( \mathcal{E} \), we can also index the identifying vector \( a \in \mathbb{R}^E \) of \( A \in K_{p,q} \) equivalently by monomials in \( \mathcal{E} \) as
\[
a = (a_\omega)_{\omega \in \mathcal{E}} \in \mathbb{R}^E, \quad \text{with } a_{x_i y_j x_k y_l} = a_{ijkl}, \quad (i,j,k,l) \in E.
\]
We call such a an $\mathcal{E}$-truncated moment sequence ($\mathcal{E}$-tms) (cf. [21]).

The $\mathcal{E}$-truncated $\Delta$-moment problem ($\mathcal{E}$-T$\Delta$MP) studies whether or not a given $\mathcal{E}$-tms $a$ admits a $\Delta$-representing measure $\mu$. A measure is called finitely atomic if its support is a finite set, and is called $r$-atomic if its support consists of at most $r$ distinct points. Let $\mu$ be the weighted sum of Dirac measures:

$$\mu := \rho_1 \delta_{(a_1,b_1)} + \cdots + \rho_r \delta_{(a_r,b_r)}.$$  

Then, (19) is equivalent to

$$a_{xi,yi,ki} = \int_{\Delta} x_i y_i k_i d\mu, \quad \forall x_i y_i k_i \in \mathcal{E}. \quad (23)$$

Thus, a matrix $A \in K_{p,q}$ is completely positive separable (i.e., $A \in \mathcal{CP}_{p,q}$) if and only if its identifying vector $a \in \mathbb{R}^\mathcal{E}$ admits a $\Delta$-measure. In other words, if we denote the cone

$$\mathcal{R}_E(\Delta) := \{ a \in \mathbb{R}^\mathcal{E} : a \text{ admits a } \Delta \text{-measure} \},$$

then $\mathcal{R}_E(\Delta)$ is the completely positive separable matrix cone $\mathcal{CP}_{p,q}$. So, we have

$$A \in \mathcal{CP}_{p,q} \quad \text{if and only if} \quad a \in \mathcal{R}_E(\Delta),$$

where $\mathcal{E}$ and $\Delta$ are given as in (20) and (17), respectively.

### 3.2. Properties of the cone $\mathcal{CP}_{p,q}$

The completely positive separable matrix cone $\mathcal{CP}_{p,q}$ can be thought of as subsets of the vector space $\mathbb{R}^\mathcal{E}$, for $\mathcal{E}$ as in (20). Denote the polynomial cone

$$\mathbb{R}[x,y]_\mathcal{E} := \text{span}\{\mathcal{E}\}.$$

We say that $\mathbb{R}[x,y]_\mathcal{E}$ is $\Delta$-full if there exists a polynomial $p(x,y) \in \mathbb{R}[x,y]_\mathcal{E}$ such that $p(x,y) > 0$ on $\Delta$. In fact, if we choose $p(x,y) = (x^T x)(y^T y) \in \mathbb{R}[x,y]_\mathcal{E}$, then $p(x,y) > 0$ on $\Delta$. So, $\mathbb{R}[x,y]_\mathcal{E}$ is $\Delta$-full. The $\Delta$-fullness is crucial for checking the completely positive separability to be discussed later.

### Proposition 1

For any positive integer numbers $p,q$, we always have

(i) $\mathcal{CP}_{p,q} \subseteq \mathcal{CP}_{pq}$;

(ii) the cone $\mathcal{CP}_{p,q}$ is a proper cone (i.e., it is closed, convex, pointed, and full-dimensional).

**Proof.** (i) Let $B \in \mathcal{CP}_p$, $C \in \mathcal{CP}_q$ and $A = B \otimes C$. Then, $B = \sum_{i=1}^r \lambda_i b_i b_i^T$ and $C = \sum_{j=1}^l \tau_j c_j c_j^T$, where $\lambda_i (i = 1, \ldots, r)$ and $\tau_j (j = 1, \ldots, l)$ are nonnegative numbers, $b_i \in \mathbb{R}_+^p$ and $c_j \in \mathbb{R}_+^q$ with $\|b_i\|_2 = \|c_j\|_2 = 1$. Using basic algebraic rules for tensor products, we obtain

$$A = B \otimes C = \left( \sum_{i=1}^r \lambda_i b_i b_i^T \right) \otimes \left( \sum_{j=1}^l \tau_j c_j c_j^T \right) = \sum_{i,j} \lambda_i \tau_j (b_i b_i^T \otimes c_j c_j^T) = \sum_{i,j} \lambda_i \tau_j (b_i \otimes c_j)(b_i \otimes c_j)^T.$$  

It is clear that each $b_i \otimes c_j \in \mathbb{R}_+^{p \times q}$ and $\lambda_i \tau_j \geq 0$ for all $i,j$. So $A \in \mathcal{CP}_{pq}$. Since a completely positive separable matrix is a nonnegative linear combination of such matrices, it follows that $\mathcal{CP}_{p,q} \subseteq \mathcal{CP}_{pq}$.

(ii) It is easy to check that $\mathcal{CP}_{p,q}$ is pointed. Note that $\Delta$ is a nonempty compact set, $\mathcal{E}$ is finite and $\mathbb{R}[x,y]_\mathcal{E}$ is $\Delta$-full. Hence, by [22, Proposition 3.2], the cone $\mathcal{CP}_{p,q}$ is proper. 

\[\square\]
4. A semidefinite relaxation algorithm for checking completely positive separability. In this section, we propose a semidefinite relaxation algorithm to check whether a given matrix $A \in \mathcal{K}_{p,q}$ is completely positive separable or not. The convergence of the algorithm is also analysed.

4.1. A semidefinite relaxation algorithm. As shown in Section 3, a matrix $A \in \mathcal{K}_{p,q}$ is completely positive separable if and only if its identifying vector $a \in \mathbb{R}^\varepsilon$ admits a $\Delta$-measure.

Let

$$h(x, y) := (x^T x - 1, y^T y - 1), \quad g(x, y) := (x, y).$$

(24)

Then the set $\Delta$ as in (17) can be rewritten as

$$\Delta := \{(x, y) \in \mathbb{R}^p \times \mathbb{R}^q : h(x, y) = 0, g(x, y) \geq 0\}.$$  

(25)

Suppose $w \in \mathbb{R}^{[x,y]2t}$ is an extension of $a$, i.e., $w|_{\varepsilon} = a$. As we show above, if $w$ is flat with respect to $h = 0$ and $g \geq 0$, i.e., it satisfies

$$L_h^{(t)}(w) = 0, L_g^{(t)}(w) \succeq 0, M_t(w) \succeq 0,$$

(26)

and the rank condition

$$\text{rank} M_{t-1}(w) = \text{rank} M_t(w),$$

(27)

then $w$ admits a unique $\Delta$-measure $\mu$, which is $r$-atomic with $r := \text{rank} M_t(w)$. In other words, there exist $\rho_i > 0, (a_i, b_i) \in \Delta(i = 1, \ldots, r)$ such that

$$w = \rho_1[(a_1, b_1)]_{2t} + \cdots + \rho_r[(a_r, b_r)]_{2t}.$$  

(28)

The extension condition $w|_{\varepsilon} = a$ and (28) imply that

$$a = \rho_1[(a_1, b_1)]_{\varepsilon} + \cdots + \rho_r[(a_r, b_r)]_{\varepsilon}.$$  

Furthermore, we can get the following CPS-decomposition for $A$:

$$A = \rho_1(a_1a_1^T) \otimes (b_1b_1^T) + \cdots + \rho_r(a_r a_r^T) \otimes (b_r b_r^T).$$  

(29)

It is clear that if there exists a flat extension of $a$, then $A$ is completely positive separable. Conversely, if $A$ is completely positive separable and if only if its identifying vector $a$ has a flat extension. Based on this, we construct the following semidefinite relaxation to check whether a given matrix is CPS or not.

Let $d > 4$ be an even integer. A polynomial in $M[x,y]_d$ is said to be generic if it is in an open dense subset of $M[x,y]_d$ in the Zariski topology. Choose a generic polynomial $F \in \Sigma[x,y]_d$. Let $h, g$ be as in (24). For relaxation orders $k \geq d/2$, consider the semidefinite relaxation

$$\begin{align*}
\min \quad & \langle F, w \rangle \\
\text{s.t.} \quad & w|_{\varepsilon} = a, L_h^{(k)}(w) = 0, L_g^{(k)}(w) \succeq 0, \\
& M_k(w) \succeq 0, w \in \mathbb{R}^{[x,y]2k}.
\end{align*}$$

(30)

The dual problem of (30) is

$$\begin{align*}
\max \quad & \langle f, a \rangle \\
\text{s.t.} \quad & F - f \in I_{2k}(h) + Q_{2k}(g), f \in \mathbb{R}[x, y]_{\varepsilon}.
\end{align*}$$

(31)

The variable in (31) is the vector of coefficients of $f$.

Based on solving the hierarchy of (30), we can propose the semidefinite relaxation algorithm for checking the membership in the cone $\mathcal{CP}_{p,q}$ as follows.
Algorithm 4.1. **Step 0.** Input $A \in K_{p,q}$ and $\Delta$ as (17). Choose a generic $F \in \Sigma[x,y]_6$. Let $k := 3$.

**Step 1.** If (30) is infeasible, then $A \notin CP_{p,q}$ and stop; otherwise, solve it for a minimizer $w^{*,k}$. Let $t := 2$.

**Step 2.** Let $z := w^{*,k}|_{2t}$. If the rank condition in (27) is not satisfied, go to Step 4.

**Step 3.** Compute $\rho_i > 0$ and $(a_i, b_i) \in \Delta$. Output the CPS-decomposition of $A$ as

$$A = (u_1 u_1^T) \otimes (v_1 v_1^T) + \cdots + (u_r u_r^T) \otimes (v_r v_r^T),$$

where $r = \text{rank}(M_t(z))$ and each $u_i = \sqrt[3]{\rho_i} a_i, v_i = \sqrt[3]{\rho_i} b_i$. Stop.

**Step 4.** If $t < k$, set $t := t + 1$ and go to Step 2; otherwise, set $k := k + 1$ and go to Step 1.

**Remark 1.** Algorithm 4.1 can be easily implemented by the software GlotpiPoly $^3$ [13], which solves the generalized problem of moments. In Step 0, we choose $F = \Sigma[x,y]_3(R^T R)[x,y]_3$, where $R$ is a random matrix of length $(p+q+3)^3$.

In Step 1, we solve the semidefinite relaxation problem (30) by the semidefinite programming solver SeDuMi. It is a Matlab toolbox for optimization over symmetric cones, based on primal-dual interior point methods [30]. The infeasibility of (30) can be certificated by the Farkas dual solution computed by the SeDuMi (cf. [30, 31]). In Step 2, we evaluate the rank of a matrix as the number of its singular values that are larger than $10^{-6}$, which is a standard procedure in numerical linear algebra [6]. In Step 3, the method in Henrion and Lasserre [12] is used to compute the finitely atomic $\Delta$-measure $\mu$ admitted by $z$, i.e., $\rho_i$ and $(a_i, b_i)$.

4.2. **Convergence of the algorithm.** We first show how to decide that $A$ is not completely positive separable, then prove the asymptotic convergence of Algorithm 4.1.

**Theorem 4.2.** Let $A \in K_{p,q}$ with its identifying vector $a$ as in (21). Then Algorithm 4.1 has the following properties:

(1) If (30) is infeasible for some $k$, then $A$ is not completely positive separable, i.e., $A \notin CP_{P,q}$.

(2) If $A \notin CP_{P,q}$, then (30) is infeasible when $k$ is big enough.

(3) If $A \in CP_{P,q}$, then for almost all generated $F$, we can asymptotically get a flat extension of $a$ by solving the hierarchy of (30).

**Proof.** Since $\mathbb{R}[x]_3$ is $\Delta$-full for the $\Sigma$ and $\Delta$ given in (20) and (25), respectively, the conclusions can be deduced from Nie [21, Section 5].

Next, we investigate when Algorithm 4.1 converges within finitely many steps. Recall that the set $\Delta$ is given in (25). Denote the polynomial cone

$$\mathcal{P}_0(\Delta) := \{ f \in \mathbb{R}[x,y]_6 : f \text{ is nonnegative on } \Delta \}.$$ 

Since $\Delta$ is compact, its dual cone is

$$\mathcal{R}_0(\Delta) := \{ z \in \mathbb{R}^{M[x,y]_6} : z \text{ admits a } \Delta\text{-measure} \}.$$ 

Consider the optimization problem

$$\max (f, a) \text{ s.t. } F - f \in \mathcal{P}_0(\Delta), f \in \mathbb{R}[x,y]_\Sigma.$$ 

(32)
Then the dual problem of (32) is
\[
\min \langle F, z \rangle \quad \text{s.t.} \quad z|_{\Delta} = a, \ z \in R_{n}(\Delta).
\] (33)

**Assumption 4.3.** Suppose \( f^* \) is a maximizer of (32), \( \hat{f} := F - f^* \in I(h) + Q(g) \) and \( \hat{f} \) has finitely many critical zeros on \( \Delta \) as in (25).

As shown in [23], if \( f \) is nonnegative on \( \Delta \), then we often have \( f \in I(h) + Q(g) \) under some general optimality conditions. So, Assumption 4.3 is generically satisfiable. Now we prove the finite convergence of Algorithm 4.1 under Assumption 4.3.

**Theorem 4.4.** Let \( A \in CP_{p,q} \) and \( a \) be as in (21). Suppose \( F \in \text{int}(\Sigma[x,y]_0) \), \( f^* \) is a maximizer of (32), and Assumption 4.3 holds. For all \( k \) sufficiently large, if \( w^{*,k} \) is a minimizer of (30), then the condition (27) must be satisfied for some \( t \geq 2 \).

**Proof.** Since \( F \in \text{int}(\Sigma[x,y]_0) \), the feasible set of (31) has an interior point. Then, for all \( k \geq 3 \), (30) is feasible and has a minimizer, and the optimization problems (30) and (31) have the same optimal values (cf. [21, Proposition 5.1]). By Assumption 4.3, it holds that \( \hat{f} := F - f^* \in I(h) + Q(g) \) and there exists \( k_1 \) such that
\[
\hat{f} \in I_{2k_1}(h) + Q_{2k_1}(g).
\]
So, for all \( k \geq k_1 \), \( f^* \) is a maximizer of (31), and
\[
\langle F, w^{*,k} \rangle = \langle f^*, a \rangle = \langle f^*, w^{*,k} \rangle.
\]
This implies that \( \langle \hat{f}, w^{*,k} \rangle = 0 \) for all \( k \geq k_1 \). The strong duality holds between (32) and (33), because \( F \in \text{int}(\Sigma[x,y]_0) \). Since \( A \in CP_{p,q} \), \( a \) admits a \( \Delta \)-measure and (33) must have a minimizer \( z^* \). Then, we have
\[
0 = \langle F, z^* \rangle - \langle f^*, a \rangle = \langle f, z^* \rangle = \int \hat{f} d\mu.
\]
where \( \mu \) is a \( \Delta \)-measure for \( z^* \). Note that \( \hat{f} \) is nonnegative on \( \Delta \). This implies that the minimum value of \( \hat{f} \) on \( \Delta \) is zero. Consider the polynomial optimization problem
\[
\min_{(x,y) \in \mathbb{R}^p \times \mathbb{R}^q} \hat{f}(x,y) \quad \text{s.t.} \quad h(x,y) = 0, \ g(x,y) \geq 0.
\] (34)
The \( k \)-th order SOS relaxation for (34) is
\[
f_{1,k} := \max \gamma \quad \text{s.t.} \quad \hat{f} - \gamma \in I_{2k}(h) + Q_{2k}(g).
\] (35)
Its dual problem is
\[
\begin{align*}
\min_{w \in \mathbb{R}^{(p+x+y)/2k}} & \quad \langle \hat{f}, w \rangle \\
\text{s.t.} & \quad 1, w = 1, M_k(w) \succeq 0, \\
& \quad L_h^{(k)}(w) = 0, L_g^{(k)}(w) \succeq 0.
\end{align*}
\] (36)
Since \( \hat{f} \in I_{2k_1}(h) + Q_{2k_1}(g) \), we have \( f_{1,k} \geq 0 \) for all \( k \geq k_1 \). On the other hand, the minimum value of \( \hat{f} \) on \( \Delta \) is 0, so \( f_{1,k} \leq 0 \) for all \( k \). Hence,
\[
f_{1,k} = 0, \quad \forall k \geq k_1.
\]
This implies that the problem (35) achieves its optimal value for \( k \geq k_1 \) and the sequence \( \{f_{1,k}\} \) has finite convergence. By Assumption 4.3, \( \hat{f} \) has finitely many critical zeros on \( \Delta \) and Assumption 2.1 in [20] for (34) is satisfied.
Example 5.2. Consider the matrix
\[
\begin{pmatrix}
5 & 0 \\
0 & 5
\end{pmatrix}
\]
Numerical experiments. Indeed, this always happens in our numerical experiments. It takes about 7 seconds, and the rank of the moment matrix is 6.

The semidefinite relaxation (30) is infeasible for \(k \geq 1\) and \(G_l \in CP\). The computation is implemented on a Lenovo Laptop with Intel Core i5-3210M 2.5 GHz and RAM 4.0 GB, using MATLAB R2014a. We use the software \texttt{GloptiPoly 3} [13] and \texttt{SeDuMi} [30] to solve semidefinite relaxations (30). We only displayed 4 decimal digits for computational results.

Example 5.1. Consider the matrix in \(S_4\)
\[
A = \begin{bmatrix}
1 & 0 & 2 & 1 \\
0 & 1 & 1 & 1 \\
2 & 1 & 1 & 0 \\
1 & 1 & 0 & 1
\end{bmatrix}
\]
The semidefinite relaxation (30) is infeasible for \(k = 3\), so \(A\) is not completely positive separable, i.e., \(A \notin CP_{2,2}\). It takes around 4 seconds.

Example 5.2. Consider the matrix \(A = A_1 + 2A_2 + A_3\) in \(K_{3,3}\), where
\[
A_1 = (e_1e_1^T) \otimes (e_1e_1^T) + (e_2e_2^T) \otimes (e_2e_2^T) + (e_3e_3^T) \otimes (e_3e_3^T),
A_2 = (e_1e_1^T) \otimes (e_2e_2^T) + (e_2e_2^T) \otimes (e_3e_3^T) + (e_3e_3^T) \otimes (e_1e_1^T),
A_3 = (e_1e_2^T + e_2e_1^T) \otimes (e_1e_2^T + e_2e_1^T) + (e_1e_3^T + e_3e_1^T) \otimes (e_1e_3^T + e_3e_1^T) + (e_2e_3^T + e_3e_2^T) \otimes (e_2e_3^T + e_3e_2^T).
\]
The semidefinite relaxation (30) is infeasible for \(k = 3\), so \(A\) is not completely positive separable, i.e., \(A \notin CP_{3,3}\). It takes about 8 seconds.

Example 5.3. Consider the Hilbert matrix \(A \in S_6\), where
\[
A_{i,j} = \frac{1}{i + j - 1}, \quad \forall 1 \leq i, j \leq 6.
\]
It was shown in [2] that every Hilbert matrix is completely positive, i.e., \(A \in CP_6\).

(i) Firstly, we check whether \(A \in CP_{3,2}\) or not. By Algorithm 4.1, we got \(A \in CP_{3,2}\) and obtained a CPS-decomposition \(A = \sum_{i=1}^6 (u_iu_i^T) \otimes (v_iv_i^T)\), where \((u_i, v_i)\) are listed by column by column as follows:

| \(u_i\) | \(v_i\) |
|---|---|
| 0.0268 | 0.5778 | 0.7738 | 0.8137 | 0.6172 | 0.1141 |
| 0.1493 | 0.0000 | 0.0559 | 0.3373 | 0.5336 | 0.0000 |
| 0.1241 | 0.0012 | 0.0020 | 0.1434 | 0.4591 | 0.1170 |
| 0.1418 | 0.5768 | 0.7519 | 0.7486 | 0.6861 | 0.0682 |
| 0.1353 | 0.0343 | 0.1910 | 0.4859 | 0.6368 | 0.1485 |

It takes about 7 seconds, and the rank of the moment matrix is 6.
(ii) Next, we check whether $A \in \mathcal{CP}_{2,3}$ or not. By Algorithm 4.1, we got $A \in \mathcal{CP}_{2,3}$ and obtained a CPS-decomposition $A = \sum_{i=1}^{5} (u_i u_i^T) \otimes (v_i v_i^T)$, where $(u_i, v_i)$ are listed column by column as follows:

| 0.7072 | 0.6764 | 0.8275 | 0.7851 | 0.0000 |
| 0.0000 | 0.0344 | 0.1667 | 0.5799 | 0.2624 |
| 0.7026 | 0.6377 | 0.6955 | 0.6186 | 0.0722 |
| 0.0804 | 0.2108 | 0.4145 | 0.5580 | 0.1464 |
| 0.0079 | 0.0864 | 0.2354 | 0.5073 | 0.2055 |

It takes about 8 seconds, and the rank of the moment matrix is 5.

**Example 5.4.** Consider the symmetric Pascal matrix $A \in \mathcal{S}_4$, where

$$A_{i,j} = \frac{(i+j-2)!}{(i-1)!(j-1)!}, \quad \forall 1 \leq i, j \leq 4.$$  

It is easy to check that $A$ is doubly nonnegative with the order 4, so $A \in \mathcal{CP}_4 = \mathcal{CP}_{4,4} = \mathcal{CP}_{4,4}$. Indeed, all Pascal matrices $A \in \mathcal{S}_n$ are completely positive matrices [18].

(i) Firstly, we verify that $A \in \mathcal{CP}_{4,4}$ by Algorithm 4.1. We got $A \in \mathcal{CP}_{4,4}$ and obtained a CPS-decomposition $A = \sum_{i=1}^{5} (u_i u_i^T) \otimes (v_i v_i^T)$, where $(u_i, v_i)$ are listed column by column as follows:

| 0.0000 | 0.5886 | 0.0000 | 0.0000 | 0.2943 |
| 0.0000 | 0.7980 | 0.0000 | 0.4400 | 0.7287 |
| 0.0829 | 0.4934 | 0.6469 | 1.2917 | 1.3531 |
| 1.5393 | 0.0000 | 2.5695 | 2.6285 | 2.0472 |
| 1.5415 | 1.1076 | 2.6497 | 2.9572 | 2.5767 |

It takes about 28 seconds.

(ii) Next, we check whether $A \in \mathcal{CP}_{2,2}$ or not. By Algorithm 4.1, the semidefinite relaxation (30) is infeasible for $k = 3$, so $A$ is not completely positive separable, i.e., $A \notin \mathcal{CP}_{2,2}$. It takes about 4 seconds.

**Example 5.5.** Consider the Lehmer matrix $A \in \mathcal{S}_n$, where

$$A_{i,j} = \min\{i, j\}, \quad \forall 1 \leq i, j \leq n.$$  

It was shown in [18] that all Lehmer matrices are completely positive. Here, we consider the case $n = 6$.

(i) Firstly, we verify that $A \in \mathcal{CP}_{6,1}$ by Algorithm 4.1. We got $A \in \mathcal{CP}_{6,1}$ and obtained a CPS-decomposition $A = \sum_{i=1}^{13} (u_i u_i^T) \otimes (v_i v_i^T)$, where $(u_i, v_i)$ are listed column by column as follows:

| 0.3669 | 0.4136 | 0.6398 | 0.0000 | 0.0000 | 0.0000 |
| 0.3669 | 0.0000 | 0.6483 | 0.4936 | 0.4622 | 0.0000 |
| 0.0000 | 0.0000 | 0.3387 | 0.0003 | 0.3624 | 0.0000 |
| 0.0000 | 0.0896 | 0.0145 | 0.3219 | 0.0004 | 0.3103 |
| 0.0000 | 0.4023 | 0.0000 | 0.0000 | 0.0000 | 0.3576 |
| 0.0000 | 0.0000 | 0.0000 | 0.0003 | 0.4151 | 0.3711 |
| 0.5146 | 0.5839 | 1.0123 | 0.5897 | 0.7195 | 0.6016 |
| 0.6626 | 0.0000 | 0.0000 | 0.0000 | 0.5142 |
| 0.0000 | 0.2675 | 0.4132 | 0.0000 | 0.2751 | 0.0000 |
| 0.0001 | 0.4021 | 0.5421 | 0.4707 | 0.4821 | 0.2992 |
| 0.1835 | 0.4022 | 0.4223 | 0.4021 | 0.5048 | 0.4944 |
| 0.3483 | 0.3550 | 0.5046 | 0.5023 | 0.0000 | 0.0000 |
| 0.4052 | 0.0000 | 0.1937 | 0.6502 | 0.0000 | 0.0000 |
| 0.8261 | 0.7569 | 0.9669 | 1.0288 | 0.7503 | 0.7720 |

It takes about 1363 seconds, and the rank of the moment matrix is 13.
(ii) Next, we check whether \( A \in CP_{2,3} \) or not. By Algorithm 4.1, the semidefinite relaxation (30) is infeasible for \( k = 3 \), so \( A \) is not completely positive separable, i.e., \( A \notin CP_{2,3} \). The computational time is around 6 second.

**Example 5.6.** Consider the matrix \( A \) in the space \( K_{2,3} \)

\[
A = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix} \otimes \begin{bmatrix} 3 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} + \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} \otimes \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix}.
\]

Obviously, \( A \) is completely positive separable. By Algorithm 4.1, we got a CPS-decomposition \( A = \sum_{i=1}^{12} (u_i u_i^T) \otimes (v_i v_i^T) \), where \((u_i, v_i)\) are listed column by column as follows:

\[
\begin{array}{cccccccccccc}
0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.7626 & 0.0001 \\
1.0740 & 1.1492 & 1.0102 & 1.3876 & 1.5915 & 1.3031 \\
0.0000 & 0.0000 & 0.3114 & 1.1784 & 0.0000 & 1.0037 \\
1.0740 & 0.1993 & 0.0521 & 0.7325 & 1.6143 & 0.6646 \\
0.0000 & 1.1318 & 0.9596 & 0.0000 & 0.7132 & 0.4987 \\
0.8260 & 0.9647 & 1.2693 & 1.5362 & 1.5258 & 0.6776 \\
1.1856 & 1.5468 & 0.0000 & 0.0000 & 0.0000 & 1.3816 \\
0.2303 & 1.5918 & 0.3491 & 0.3407 & 1.3682 & 1.1165 \\
0.0676 & 0.8884 & 0.0000 & 1.3599 & 0.6753 & 0.8366 \\
1.4248 & 0.0000 & 1.1671 & 0.6280 & 0.0000 & 0.6492
\end{array}
\]

It takes about 26 seconds.

**Example 5.7.** Consider the matrix \( A \) in the space \( K_{3,3} \)

\[
A = I_3 \otimes I_3 + (e_1 e_1^T) \otimes (e_2 e_2^T) + (e_2 e_2^T) \otimes (e_3 e_3^T) + (e_3 e_3^T) \otimes (e_1 e_1^T).
\]

It is completely positive separable. By Algorithm 4.1, we got a CPS-decomposition \( A = \sum_{i=1}^{9} (u_i u_i^T) \otimes (v_i v_i^T) \), where \((u_i, v_i)\) are listed column by column as follows:

\[
\begin{array}{cccccccccccc}
0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.1892 & 1.0000 & 1.0000 \\
1.0000 & 0.0000 & 1.0000 & 1.1892 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 1.0000 & 0.0000 & 0.0000 & 1.1892 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 1.0000 & 0.0000 & 1.1892 & 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.0000 \\
1.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.1892 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 1.1892 & 0.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 & 1.0000
\end{array}
\]

It takes about 10 seconds.

In the following, we consider some randomly generated separable matrices.

**Example 5.8.** Consider the matrix \( A \) in the space \( K_{4,4} \)

\[
A = \sum_{i=1}^{6} (a_i a_i^T) \otimes (b_i b_i^T),
\]

where \((a_i, b_i), i = 1, \ldots, 6\) are given column by column as

\[
\begin{array}{cccccccc}
0 & 1 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 \\
1 & 1 & 1 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 1 & 1 \\
0 & 0 & 1 & 0 & 1 & 1 \\
1 & 0 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 1 & 1 & 1
\end{array}
\]
Clearly, $A$ is completely positive separable. By Algorithm 4.1, we get a CPS-decomposition $A = \sum_{i=1}^{6} (u_i u_i^T) \otimes (v_i v_i^T)$, where $(u_i, v_i)$ are listed by column as follows:

|       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|
| 0.7598 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0746 |
| 0.7598 | 0.0000 | 1.1067 | 1.1067 | 0.0000 | 0.0000 |
| 0.0000 | 0.0000 | 0.0000 | 1.1067 | 1.1892 | 1.0746 |
| 0.7598 | 1.1892 | 1.1067 | 0.0000 | 0.0000 | 1.0746 |
| 1.3161 | 0.0000 | 0.0936 | 0.0936 | 0.0000 | 0.9306 |
| 0.0000 | 0.8409 | 0.0000 | 0.0936 | 0.0000 | 0.9306 |
| 0.0000 | 0.0000 | 0.0936 | 0.0000 | 0.8409 | 0.9306 |
| 0.0000 | 0.8409 | 0.0936 | 0.0000 | 0.8409 | 0.9306 |

It takes about 140 seconds to get the CPS-decomposition, and the rank of the moment matrix is 6. The computed CPS-decomposition is the same as the input one, up to a permutation and scaling of $u_i, v_i$. That is, there exist real numbers $\tau_{i,j}$, with $i = 1, \ldots, 6$ and $j = 1, 2$ such that each $|\tau_{i,1}\tau_{i,2}| = 1$ and

$$a_i = \tau_{i,1} u_{\sigma_i}, b_i = \tau_{i,2} v_{\sigma_i},$$

In the above, the permutation vector is $\sigma = (2, 3, 1, 5, 4, 6)$.

**Example 5.9.** Consider the matrix $A$ in the space $K_{4,5}$

$$A = \sum_{i=1}^{4} (a_i a_i^T) \otimes (b_i b_i^T),$$

where $(a_i, b_i), i = 1, \ldots, 4$ are given column by column as

|       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|
| 0.4542 | 0.0016 | 0.5775 | 0.0456 |
| 0.3727 | 0.5883 | 0.9292 | 0.9070 |
| 0.8559 | 0.0364 | 0.2605 | 0.7212 |
| 0.5427 | 0.3967 | 0.3562 | 0.8369 |
| 0.0354 | 0.8269 | 0.0888 | 0.2723 |
| 0.1968 | 0.6417 | 0.7039 | 0.0270 |
| 0.9951 | 0.6516 | 0.2293 | 0.0178 |
| 0.9170 | 0.7723 | 0.9655 | 0.7830 |
| 0.0873 | 0.2373 | 0.8726 | 0.5267 |

Clearly, $A$ is completely positive separable. By Algorithm 4.1, we get a CPS-decomposition $A = \sum_{i=1}^{4} (u_i u_i^T) \otimes (v_i v_i^T)$, where $(u_i, v_i)$ are listed by column as follows:

|       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|
| 0.4913 | 0.0023 | 0.6512 | 0.0378 |
| 0.4031 | 0.8474 | 1.0477 | 0.7518 |
| 0.9258 | 0.0524 | 0.2937 | 0.5978 |
| 0.5870 | 0.5714 | 0.4016 | 0.6937 |
| 0.0327 | 0.5741 | 0.0788 | 0.3285 |
| 0.1819 | 0.4455 | 0.6243 | 0.0326 |
| 0.9199 | 0.4524 | 0.2034 | 0.0215 |
| 0.8477 | 0.5362 | 0.8563 | 0.9446 |
| 0.0807 | 0.1647 | 0.7739 | 0.6354 |

It takes about 613 seconds, and the rank of the moment matrix is 4. The computed CPS-decomposition is the same as the input one, up to a scaling of $u_i, v_i$. That is, there exist real numbers $\tau_{i,j}$, with $i = 1, \ldots, 4$ and $j = 1, 2$ such that each $|\tau_{i,1}\tau_{i,2}| = 1$ and

$$a_i = \tau_{i,1} u_i, b_i = \tau_{i,2} v_i.$$
6. Summary and discussions. In this paper, we introduce the completely positive separable matrices, which have wide applications in biquadratic polynomial optimization problem. A semidefinite algorithm is proposed for checking whether a matrix is CPS or not. If it is not CPS, a certificate for this can be obtained; if it is CPS, a CPS-decomposition can be obtained. Computational results show that the algorithm is efficient at checking CPS.

As mentioned in Section 1, completely positive separable matrices have important applications in biquadratic polynomial optimization, which arises from the strong ellipticity condition problem in solid mechanics (for \( p = q = 3 \)) [28, 29, 32], the entanglement problem in quantum physics [5, 10], as well as the best rank-one tensor approximation [26, 27]. In practice, it is often desirable to solve the biquadratic polynomial optimization with nonnegative variable constraints, stated as

\[
\begin{align*}
\min & \quad \sum_{1 \leq i,j,k,l \leq q} b_{ijkl}x_iy_jx_ky_l \\
\text{s.t.} & \quad x^T x = 1, y^T y = 1, \\
& \quad x \in \mathbb{R}^+_{p}, y \in \mathbb{R}^+_{q}.
\end{align*}
\]

Without loss of generality, we assume that the coefficients \( b_{ijkl} \) satisfy the symmetric property, i.e, \( b_{ijkl} = b_{klij} = b_{ikjl} \) for \( i, k, l = 1, \ldots, q \).

Let \( B \in S_{pq} \) be a symmetric matrix with elements \( B_{(i-1)q+j,(k-1)q+l} = b_{ijkl}, \) \( \forall 1 \leq i, k \leq p, 1 \leq j, l \leq q. \)

Then we have

\[
\sum_{1 \leq i,k \leq p, 1 \leq j,l \leq q} b_{ijkl}x_iy_jx_ky_l = \langle B, xx^T \otimes yy^T \rangle.
\]

Clearly, the problem (37) is equivalent to

\[
\begin{align*}
\min & \quad \langle B, xx^T \otimes yy^T \rangle \\
\text{s.t.} & \quad \langle I_{pq}, xx^T \otimes yy^T \rangle = 1, \\
& \quad x^T x = 1, y^T y = 1, \\
& \quad x \in \mathbb{R}^+_{p}, y \in \mathbb{R}^+_{q},
\end{align*}
\]

where \( I_{pq} \) is the identity matrix.

Then, the relaxation problem of (38) can be obtained as follows:

\[
\begin{align*}
\min & \quad \langle B, Z \rangle \\
\text{s.t.} & \quad \langle I_{pq}, Z \rangle = 1, Z \in CP_{p,q}.
\end{align*}
\]

It is clear that \( v_{BIQ}^* \geq v_{CP}^* \). In fact, we can prove that the problems (37) and (39) have the same optimal value, i.e., \( v_{BIQ}^* = v_{CP}^* \).

**Theorem 6.1.** Let \( \Delta \) be as in (25) and \( Z^* \in CP_{p,q} \) be an optimal solution of the problem (39). Then there exists \( (x^*, y^*) \in \Delta \) such that \( \langle B, Z^* \rangle = \langle B, xx^T \otimes y^*y^T \rangle \), that is, we have \( v_{BIQ}^* = v_{CP}^* \).

**Proof.** Since \( Z^* \in CP_{p,q} \) is an optimal solution of the problem (39), we always have \( \langle B, Z^* \rangle \leq \langle B, xx^T \otimes yy^T \rangle \) for any \( (x, y) \in \Delta \). In the following, we show that there exists a vector \( (x^*, y^*) \in \Delta \) such that \( \langle B, Z^* \rangle \geq \langle B, xx^T \otimes y^*y^T \rangle \).

Because \( Z^* \in CP_{p,q} \), there exist \( \rho_1, \ldots, \rho_r > 0 \) and \( (a_1, b_1), \ldots, (a_r, b_r) \in \Delta \) such that

\[
Z^* = \sum_{s=1}^r \rho_s (a_s a_s^T) \otimes (b_s b_s^T).
\]
Without loss of generality, we assume that
\[ \langle B, (a_1 a_1^T) \otimes (b_1 b_1^T) \rangle \leq \langle B, (a_2 a_2^T) \otimes (b_2 b_2^T) \rangle \leq \ldots \leq \langle B, (a_r a_r^T) \otimes (b_r b_r^T) \rangle. \]
Then we have
\[ 1 = \langle I_{pq}, Z^* \rangle = \langle I_{pq}, \sum_{s=1}^r \rho_s (a_s a_s^T) \otimes (b_s b_s^T) \rangle = \sum_{s=1}^r \rho_s \langle I_{pq}, (a_s a_s^T) \otimes (b_s b_s^T) \rangle = \sum_{s=1}^r \rho_s. \]
Therefore,
\[ \langle B, Z^* \rangle = \langle B, \sum_{s=1}^r \rho_s (a_s a_s^T) \otimes (b_s b_s^T) \rangle = \sum_{s=1}^r \rho_s \langle B, (a_s a_s^T) \otimes (b_s b_s^T) \rangle \geq \sum_{s=1}^r \rho_s \langle B, (a_1 a_1^T) \otimes (b_1 b_1^T) \rangle = \langle B, (a_1 a_1^T) \otimes (b_1 b_1^T) \rangle. \]
Let \( (x^*, y^*) = (a_1, b_1) \), then \( \langle B, Z^* \rangle = \langle B, x^* x^T \otimes y^* y^T \rangle \), i.e., \( v^*_{B_{IQ}} = v_{CPS}^* \). This completes the proof. \( \square \)

Theorem 6.1 implies that the biquadratic polynomial optimization problem (37) is equivalent to the completely positive separable cone problem (39). Moreover, all the vectors \( (a_1, b_1), \ldots, (a_r, b_r) \in \Delta \) satisfying (40) are optimal solutions of the problem (37). To design efficient numerical methods for solving (39), one needs to check the memberships in \( CP_{p,q} \). Thus, a method similar to Algorithm 4.1 can be designed to solve (39).

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