APPROXIMATE COMPLETELY POSITIVE SEMIDEFINITE RANK

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Abstract. In this paper we provide an approximation for *completely positive semidefinite (cpsd)* matrices with cpsd-rank bounded above (almost) independently from the cpsd-rank of the initial matrix. This is particularly relevant since the cpsd-rank of a matrix cannot, in general, be upper bounded by a function only depending on its size.

For this purpose, we make use of the Approximate Carathéodory Theorem in order to construct an approximate matrix with a low-rank Gram representation. We then employ the Johnson-Lindenstrauss Lemma to improve to a logarithmic dependence of the cpsd-rank on the size.

1. Introduction

The maximal angle between vectors from some nonnegative orthant $\mathbb{R}_+^d$ is $\pi/2$. If finitely many such nonnegative vectors $v_1, \dots, v_n$ are given, the (entrywise nonnegative) matrix

$$M = \left(\langle v_i, v_j \rangle\right)_{i,j=1,\dots,n}$$

is called a *completely positive matrix.* So the possible combinations of angles between tuples of nonnegative vectors is encoded in the convex cone of all completely positive matrices. The cone of completely positive matrices has numerous applications in control theory and general optimization, among others. It has been intensively studied, see for example [2].

When putting a nonnegative vector on the diagonal of a quadratic matrix, one obtains a special *positive semidefinite matrix.* Now a canonical non-commutative/quantum generalization of completely positive matrices arises by choosing $A_1, \dots, A_n$ from some cone of positive semidefinite matrices, and considering the matrix

$$M = \left(\langle A_i, A_j \rangle\right)_{i,j=1,\dots,n}$$

where we use the trace inner product for matrices. Such matrices are called *completely positive semidefinite.* So the cone of completely positive semidefinite matrices encodes the possible angles between tuples of positive semidefinite matrices. These cones allow for a conic optimization approach to quantum correlations and quantum graph colorings, for example [9, 11].

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Note that the angle between two general positive semidefinite matrices is also at most $\pi/2$, so both completely positive and completely positive semidefinite matrices have non-negative entries.

As it happens often, the non-commutative/quantum analogue is much more challenging to understand than the commutative/classical version. For example, the cone of completely positive matrices is closed, whereas the cone of completely positive semidefinite matrices have recently been shown not to be closed in general [5, 11, 16]. Also, to both kinds of decompositions there is an associated rank, measuring the minimal size of the nonnegative vectors/positive semidefinite matrices that are necessary to represent the given matrix. Whereas the *completely positive rank* can be bounded in terms of the size n alone, this fails for the *completely positive semidefinite rank*, as we will explain below. This significant difference serves as the main motivation for this paper.

Our main result yields an approximation of completely positive semidefinite matrices of relatively small completely positive semidefinite rank. This rank of the approximation depends on the size n, the accuracy of the approximation, and a certain complexity of the initial matrix. However, most importantly, it does not depend on its completely positive semidefinite rank. We provide two such results, one being better for fixed approximation error and n very large, the other better for fixed n and small approximation error.

The main ingredients of our proof are the *Approximate Carathéodory Theorem* and the *Johnson-Lindenstrauss Lemma*. We will first approximate the initial matrix, using the Approximate Carathéodory Theorem. This application will already establish the first upper bound. In a second step, we will then further improve the approximation by applying the Johnson-Lindenstrauss Lemma to the eigendecomposition of the positive semidefinite matrices in the representation. This will reduce the linear dependence on n of the upper bound to a logarithmic dependence, and so establish the second upper bound.

Section 2 contains the essential preliminary material and an explanation of the fact why the completely positive semidefinite rank cannot be bounded by n alone. Section 3 then contains our main result and some examples.

2. Notations and preliminaries

We will first state some basic definitions and results used throughout this paper. Let $[n]$ be the set $\{1, \ldots, n\}$ and $\mathcal{S}^n$ be the space of all $n \times n$ real symmetric matrices (i.e. $A^t = A$) endowed with the trace inner product:

$$\langle A, B\rangle = \operatorname{tr}(BA) = \sum_{i,j=1}^{n} A_{ij} B_{ij}.$$

The corresponding norm is known as the Frobenius norm: $\|A\|_{\mathcal{F}} = \sqrt{\langle A, A\rangle}$.

A non-empty subset $\mathcal{C} \subseteq \mathcal{S}^n$ is called a *convex cone* if it is closed under nonnegative linear combinations, i.e. for all $\alpha, \alpha' \geqslant 0$ and for all $c, c' \in \mathcal{C}$ we have $\alpha c + \alpha' c' \in \mathcal{C}$. Moreover, $\mathcal{C}$ is called *pointed*, *full-dimensional* and *closed*, respectively, if $\mathcal{C} \cap -\mathcal{C} = \{0\}$, if it has a non-empty interior and if it is a closed set in the Euclidean topology, respectively. We call a convex cone with these three properties a *proper* cone. Given a convex cone $\mathcal{C} \subseteq \mathcal{S}^n$, its dual cone is defined as

$$\mathcal{C}^* \coloneqq \{A \in \mathcal{S}^n : \langle A, B\rangle \geqslant 0 \quad \text{for all } B \in \mathcal{C}\}$$

and this is always a closed convex cone.

A real symmetric matrix $A \in \mathcal{S}^n$ is called *positive semidefinite* (*psd* for short, and denoted by $A \succcurlyeq 0$) if there exist vectors $v_1, \ldots, v_n \in \mathbb{R}^d$, for some $d \in \mathbb{N}$, such that $A = (\langle v_i, v_j\rangle)_{i,j=1}^n$, where $\langle \cdot, \cdot \rangle$ denotes the standard inner product on $\mathbb{R}^d$. We also say that the vectors $v_1, \ldots, v_n$ form a *Gram representation* of A. It is well-known that the smallest possible d in a Gram representation of A coincides with its usual matrix rank $\operatorname{rank}(A)$. We denote by $\mathcal{S}_+^n$ the set of all $n \times n$ positive semidefinite matrices and it is well-known that it is a proper and self-dual cone, i.e., $\mathcal{S}_+^n = (\mathcal{S}_+^n)^*$.

A real symmetric matrix $A \in \mathcal{S}^n$ is called *doubly nonnegative* if it is both positive semidefinite and entrywise nonnegative. So this means that it admits a Gram representation by vectors $v_1, \ldots, v_n \in \mathbb{R}^d$, for which the pairwise angles between the v_i does not exceed $\pi/2$, i.e. $\langle v_i, v_j\rangle \geqslant 0$ for all $i, j \in [n]$. The set of all $n \times n$ doubly nonnegative matrices is known to form a proper cone, which is denoted by $\mathcal{DNN}^n$.

A real symmetric matrix $A \in \mathcal{S}^n$ which has a Gram representation by entrywise nonnegative vectors $v_1, \ldots, v_n \in \mathbb{R}_+^d$, for some $d \in \mathbb{N}$, is called *completely positive* (*cp* for short). The smallest possible such d is known as the *cp-rank* of A. It seems that the best general upper bound on the cp-rank of an $n \times n$ cp-matrix is

$$\binom{n+1}{2} - 4$$

see [15]. The difference of this upper bound to the best known lower bound has recently been improved to $\mathcal{O}(n \log\log n)$, see [13]. The set of all $n \times n$ completely positive matrices also forms a proper cone, denoted by $\mathcal{CP}^n$. The structure of the cone $\mathcal{CP}^n$ has been extensively studied (see for example [2]). Since every nonnegative vector can be considered as a diagonal psd matrix, every cp matrix $A \in \mathcal{CP}^n$ can also be written as

$$A = (\langle x_i, x_j\rangle)_{i,j=1}^n = (\langle D_i, D_j\rangle)_{i,j=1}^n,$$

where D_i is the $d \times d$ matrix with x_i as its diagonal. In particular, every D_i is a positive semidefinite matrix. At this point, it is natural to pass from diagonal psd matrices to general psd matrices. In this way, we obtain the cone of *completely positive semidefinite* matrices.

Definition 1. A matrix $A \in \mathcal{S}^n$ is called *completely positive semidefinite* (*cpsd* for short), if it admits a Gram representation by psd matrices $A_1, \ldots, A_n \in \mathcal{S}_+^d$, for some $d \geqslant 1$, meaning

$$A = (\langle A_i, A_j\rangle)_{i,j=1}^n .$$

We denote the set of all $n \times n$ completely positive semidefinite matrices by $\mathcal{CPSD}^n$.

Lemma 2. *The set $\mathcal{CPSD}^n$ is a convex cone.*

Proof. Fix $\lambda \geqslant 0$ and let $A \in \mathcal{CPSD}^n$ with Gram representation $A_1, \ldots, A_n \in \mathcal{S}_+^d$. Then consider the psd matrices $\sqrt{\lambda}A_1, \ldots, \sqrt{\lambda}A_n \in \mathcal{S}_+^d$, which clearly form a Gram representation of the matrix λA. Therefore $\lambda A \in \mathcal{CPSD}^n$.

Now let A be as before and let $B \in \mathcal{CPSD}^n$ be another cpsd matrix with Gram representation given by $B_1, \ldots, B_n \in \mathcal{S}_+^{d'}$ for some $d' \in \mathbb{N}$. Now consider the matrices $A_1 \oplus B_1, \ldots, A_n \oplus B_n \in \mathcal{S}_+^{d+d'}$, where

$$A_i \oplus B_i \coloneqq \begin{pmatrix} A_i & 0 \\ 0 & B_i \end{pmatrix}$$

denotes the block-diagonal sum of A_i and B_i for each $i \in [n]$. For $i, j \in [n]$ we clearly have

$$(A + B)_{ij} = A_{ij} + B_{ij} = \langle A_i, A_j \rangle + \langle B_i, B_j \rangle = \langle A_i \oplus B_i, A_j \oplus B_j \rangle,$$

which proves $A + B \in \mathcal{CPSD}^n$. □

By definition, every completely positive matrix is also completely positive semidefinite. Moreover, since the trace inner product of two psd matrices is nonnegative and every psd matrix in the Gram representation of a cpsd matrix can be considered as a vector (by stacking the columns on top of each other), we obtain the following inclusions:

$$\mathcal{CP}^n \subseteq \mathcal{CPSD}^n \subseteq \mathcal{DNN}^n. \tag{1}$$

In addition, the cone $\mathcal{CPSD}^n$ is pointed and full-dimensional, which directly follows from the facts that the cone $\mathcal{DNN}^n$ is pointed and the cone $\mathcal{CP}^n$ is full-dimensional, respectively. One of the challenging questions about the cone $\mathcal{CPSD}^n$ is whether it is closed. For $n \leqslant 4$, it is known that $\mathcal{CP}^n = \mathcal{CPSD}^n = \mathcal{DNN}^n$ (first proven in [10]), and hence $\mathcal{CPSD}^n$ is closed. On the other hand, for $n \geqslant 5$ both inclusions above are strict (see [6] and [7]). Furthermore, by characterization of the closure of $\mathcal{CPSD}^n$-cone given in [4], together with the example in [7], the chain of inclusions above can even be refined to (also shown in [9])

$$\mathcal{CP}^n \subsetneq \mathcal{CPSD}^n \subseteq \mathrm{cl}(\mathcal{CPSD}^n) \subsetneq \mathcal{DNN}^n.$$

A recent breakthrough is [16], where it is shown that a certain affine section of the completely positive semidefinite cone is not closed, and hence the same holds for the cone $\mathcal{CPSD}^n$ itself, for $n \geqslant 1942$. The lower bound on n was improved in [5], where it was subsequently shown that $\mathcal{CPSD}^n$ is not closed even for $n \geqslant 10$. Hence, it remains an open problem whether the cone is closed for $n \in \{5, 6, 7, 8, 9\}$.

As the $\mathcal{CPSD}^n$-cone is a generalization of the $\mathcal{CP}^n$-cone, it is also natural to extend the notion of rank in the latter cone by replacing the nonnegative vectors with psd matrices.

Definition 3. The *completely positive semidefinite rank* of a matrix $A \in \mathcal{CPSD}^n$, denoted by cpsd-rank(A), is the smallest $d \geqslant 1$ for which there exist psd matrices $A_1, \ldots, A_n \in \mathcal{S}_+^d$ such that

$$A = (\langle A_i, A_j \rangle)_{i,j=1}^n.$$

Remark 4. Instead of using real symmetric psd matrices $A_1, \ldots, A_n \in \mathcal{S}_+^d$ in the Gram representation of cpsd-matrices, one can also use complex Hermitian matrices $A_1, \ldots, A_n \in$

$\mathcal{H}_+^d$. This gives rise to the same notion of cpsd-matrices, only decreases the cpsd-rank by a factor of at most two. This can be seen by using the isometry

$$\mathcal{H}^d \longrightarrow \mathcal{S}^{2d}; \quad M \longmapsto \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{Re}(M) & -\mathrm{Im}(M) \\ \mathrm{Im}(M) & \mathrm{Re}(M) \end{pmatrix}$$

which preserves positive semidefiniteness. We will restrict to the case of real symmetric psd matrices from now on.

In the following, we introduce another notion of rank for cpsd-matrices, which will be used in the proof of our main result.

Definition 5. Let $A \in \mathcal{CPSD}^n$. We define the *Gram-cpsd-rank* of A (denoted cpsd-rank$_{\mathfrak{G}}(A)$) as the smallest $r \geqslant 1$ for which there exists a Gram representation $A_1, \ldots, A_n \in \mathcal{S}_+^d$, for some $d \in \mathbb{N}$, with $\mathrm{rank}(A_i) \leqslant r$ for all $i \in [n]$.

The next lemma shows the relationship between the two notions of cpsd-ranks. The result is similar to Lemma 2.1 in [8] and Lemma 5 in [11], we include a proof for completeness.

Lemma 6. *Let $A \in \mathcal{CPSD}^n$. The following chain of inequalities holds:*

$$\textit{cpsd-rank}_{\mathfrak{G}}(A) \leqslant \textit{cpsd-rank}(A) \leqslant n \cdot \textit{cpsd-rank}_{\mathfrak{G}}(A).$$

Proof. The first inequality is clear from the fact that the rank of a matrix is at most its size. For the second let $A_1, \ldots, A_n \in \mathcal{S}_+^d$ be a Gram representation of $A \in \mathcal{CPSD}^n$ with $\mathrm{rank}(A_i) \leqslant \text{cpsd-rank}_{\mathfrak{G}}(A)$ for all $i \in [n]$. Then the rank r of the matrix

$$A' := \sum_{i=1}^n A_i \in \mathcal{S}_+^d$$

is at most $n \cdot \text{cpsd-rank}_{\mathfrak{G}}(A)$. By the spectral theorem we obtain

$$A' = O\mathrm{Diag}(\lambda_1, \ldots, \lambda_r, 0, \ldots, 0)O^t = ODO^t$$

for some orthogonal matrix O and $\lambda_i > 0$ for all $i \in [r]$. Now we have

$$\langle O^t A_i O, O^t A_j O\rangle = \mathrm{Tr}(O^t A_j O O^t A_i O) = \mathrm{Tr}(A_j A_i) = \langle A_i, A_j\rangle = A_{ij},$$

thus the matrices $O^t A_1 O, \ldots, O^t A_n O \in \mathcal{S}_+^d$ form a Gram representation for A as well. From the fact that $O^t A_i O \succcurlyeq 0$ for all $i \in [n]$, and

$$\sum_{i=1}^n O^t A_i O = O^t A' O = \begin{pmatrix} D_{r\times r} & 0 \\ 0 & 0 \end{pmatrix}$$

it easily follows that each $O^t A_i O$ has nonzero entries only in the upper left $r \times r$-block as well. When restricting to this upper left block we obtain a Gram representation of A with psd matrices of size r, which shows that $\text{cpsd-rank}(A) \leqslant r \leqslant n \cdot \text{cpsd-rank}_{\mathfrak{G}}(A)$. □

As we have already seen above, the cpsd-rank is a natural non-commutative analogue of the cp-rank. However, while the cp-rank is upper bounded by a function that depends only on the matrix size, there is no general such upper bound on the cpsd-rank. There are only some classes of completely positive semidefinite matrices for which there exists an upper bound in terms of the matrix size. For instance, the authors in [11] and [8] construct cpsd matrices of size $2n$ and $4n^2+2n+2$ for all $n \geqslant 1$ with cpsd-rank being $2^{\Omega(\sqrt{n})}$ and 2^n, respectively. We now explain why this is impossible in general (for $n \geqslant 10$). This observation follows directly from the non-closedness of the cpsd-cone, and is the main motivation for the results in this paper. By the definition of the $\mathcal{CPSD}^n$-cone, going through larger and larger size of the psd matrices in a Gram representation is a procedure to produce all completely positive semidefinite matrices, and so we have

$$\mathcal{CPSD}^n = \bigcup_{r\in\mathbb{N}} \mathcal{CPSD}^n_{\leqslant r},$$

where

$$\mathcal{CPSD}^n_{\leqslant r} \coloneqq \{A = \left(\langle A_i, A_j\rangle\right)_{i,j} \mid A_1,\ldots,A_n \in \mathcal{S}^r_+\}.$$

Note that we have

$$\mathcal{CPSD}^n_{\leqslant r} \subseteq \mathcal{CPSD}^n_{\leqslant r+1}$$

for all r, since psd matrices of size r can be enlarged to size $r+1$ without changing the inner product, by adding a zero row and column.

Lemma 7. *For each $n, r \geqslant 1$, the set $\mathcal{CPSD}^n_{\leqslant r}$ is closed and semialgebraic.*

Proof. Fix $n, r \geqslant 1$. Let $\left(A^{(k)}\right)_{k\in\mathbb{N}}$ be a sequence of matrices in $\mathcal{CPSD}^n_{\leqslant r}$ converging to some $A \in \mathcal{S}^n$, which clearly means $\lim_{k\to\infty} A^{(k)}_{ij} = A_{ij}$ for all $i,j \in [n]$. Now for each $k \in \mathbb{N}$ there exist $A^{(k)}_1,\ldots,A^{(k)}_n \in \mathcal{S}^r_+$ such that

$$A^{(k)}_{ij} = \operatorname{tr}\left(A^{(k)}_i A^{(k)}_j\right).$$

The converging sequence $\left(A^{(k)}\right)_k$ is bounded, in particular, all the diagonal entries

$$A^{(k)}_{ii} = \operatorname{tr}\left(A^{(k)}_i A^{(k)}_i\right) = \left\|A^{(k)}_i\right\|^2$$

are bounded. So without loss of generality, by using the Bolzano-Weierstrass Theorem and the fact that $\mathcal{S}^r_+$ is closed, we can assume that for each $i \in [n]$ the sequence $\left(A^{(k)}_i\right)_k$ converges to some $A_i \in \mathcal{S}^r_+$, and hence for each $i,j \in [n]$ we have

$$\operatorname{tr}(A_iA_j) = \lim_{k\to\infty} \operatorname{tr}\left(A^{(k)}_i A^{(k)}_j\right) = \lim_{k\to\infty} A^{(k)}_{ij} = A_{ij}.$$

This shows that $A_1,\ldots,A_n \in \mathcal{S}^r_+$ form a Gram representation for A, and thus $A \in \mathcal{CPSD}^n_{\leqslant r}$. This proves closedness.

The membership of matrices in $\mathcal{CPSD}^n_{\leqslant r}$ can be stated as a first order formula in the language of ordered rings, using quantifiers. Indeed, the existence of the Gram representation is an existential formula, since the size of the A_i is bounded by r (the quantification is over the entries of the A_i). By quantifier elimination (see for example [12]) we conclude that the set $\mathcal{CPSD}^n_{\leqslant r}$ is indeed semialgebraic. □

Corollary 8. *For $n \geqslant 10$ the cpsd-rank of elements from $\mathcal{CPSD}^n$ are unbounded.*

Proof. If the cpsd-rank admitted a bound, there would exist some $r \geqslant 1$ with $\mathcal{CPSD}^n = \mathcal{CPSD}^n_{\leqslant r}$. Consequently, by Lemma 7, the cone $\mathcal{CPSD}^n$ would be closed, which was shown to fail in [5, 16] for $n \geqslant 10$. □

To prove our main result, we make use of an approximate version of Carathéodory's Theorem [1] and a variant of the Johnson-Lindenstrauss Lemma [17]. For a set $P \subseteq \mathbb{R}^d$ we denote by $\mathrm{conv}(P)$ the convex hull of P. Further, for $k \in \mathbb{N}$ we denote the set of all convex combinations from P of length at most k by $\mathrm{conv}_k(P)$. The (exact) Carathéodory Theorem states that every element in a convex hull can be written as a convex combination of at most $d+1$ elements. Hence, we have the following increasing chain of sets:

$$P = \mathrm{conv}_1(P) \subseteq \mathrm{conv}_2(P) \subseteq \cdots \subseteq \mathrm{conv}_{d+1}(P) = \mathrm{conv}(P).$$

We now state an approximate version of Carathéodory's Theorem with respect to the 2-norm [1].

Theorem 9 (Approximate Carathéodory Theorem)**.** *Let $P \subseteq \mathbb{R}^d$ be a bounded set and $\varepsilon > 0$. Then for*

$$k = \left\lceil \frac{diam(P)^2}{2\varepsilon^2} \right\rceil$$

the set $\mathrm{conv}_k(P)$ is ε-dense in $\mathrm{conv}(P)$, meaning that for each $a \in \mathrm{conv}(P)$ there exists some $b \in \mathrm{conv}_k(P)$ such that $\|a-b\|_2 < \varepsilon$.

Since entrywise 2-norm and Hilbert-Schmidt norm for matrices coincide, this directly leads to the following rank approximation result for positive semidefinite matrices:

Corollary 10. *Let $A \in \mathcal{S}^d_+$. Then for every $\varepsilon > 0$ there exists a positive semidefinite matrix $B \in \mathcal{S}^d_+$ such that*

$$\mathrm{tr}(B) = \mathrm{tr}(A),$$

$$\|A - B\|_2 = \sqrt{\mathrm{tr}\left((A-B)^2\right)} < \varepsilon,$$

and

$$\mathrm{rank}(B) \leqslant \left\lceil \frac{\mathrm{tr}(A)^2}{\varepsilon^2} \right\rceil .$$

Proof. Consider the set

$$P := \left\{ \mathrm{tr}(A) \cdot uu^t : u \in \mathbb{R}^d, \|u\|_2 = 1 \right\} \subseteq \mathcal{S}^d_+.$$

By the eigenvalue decomposition of A it is immediate that $A \in \mathrm{conv}(P)$. Further, it is easy to check that

$$\mathrm{diam}(P) = \sqrt{2}\mathrm{tr}(A),$$

and thus Theorem 9 implies the existence of some B with

$$\sqrt{\operatorname{tr}\left((A-B)^2\right)} = \|A-B\|_2 < \varepsilon$$

which is a convex combination of at most

$$k = \left\lceil \frac{\operatorname{tr}(A)^2}{\varepsilon^2} \right\rceil$$

elements from P. Since each element in P is psd of rank 1 its trace is equal to $\operatorname{tr}(A)$, this finishes the proof. □

We will later also use the following version of the Johnson-Lindenstrauss Lemma [17]:

Theorem 11 (Johnson-Lindenstrauss Lemma)**.** *Let* $0 < \varepsilon < 1$, $\{x_1, \dots, x_m\} \subseteq \mathbb{R}^d$, *and set* $r := \left\lceil 8\log(m+1)/\varepsilon^2 \right\rceil$. *Then there exists a linear map* $Q : \mathbb{R}^d \to \mathbb{R}^r$ *such that*

$$|x_i^t x_j - x_i^t Q^t Q x_j| \leqslant \varepsilon \left(\|x_i\|_2^2 + \|x_j\|_2^2 - x_i^t x_j \right) \quad \textit{for all } i, j \in [m].$$

3. Main Result

We are now ready to state and prove our main result:

Theorem 12. *Let* $M = (\langle A_i, A_j \rangle)_{i,j=1}^n \in \mathcal{CPSD}^n$, *set* $\ell := \max_i \operatorname{tr}(A_i)$ *and* $L := \max_i M_{ii}$. *Then for every* $0 < \varepsilon < \frac{1}{2}\min\{\ell^2, L\}$ *there exists some* $N \in \mathcal{CPSD}^n$ *with*

$$\textit{cpsd-rank}(N) \leqslant \min \left\{ n \left\lceil \frac{9L\ell^2}{2\varepsilon^2} \right\rceil, \frac{(6\ell)^4 \log\left(n \left\lceil \frac{18L\ell^2}{\varepsilon^2} \right\rceil + 1 \right)}{\varepsilon^2} \right\}$$

and

$$|M_{ij} - N_{ij}| < \varepsilon \quad \textit{for all } i, j \in [n].$$

Proof. By Corollary 10, for every $i \in [n]$ there exists a psd matrix $A_i' \in \mathcal{S}_+^d$ with $\operatorname{tr}(A_i') = \operatorname{tr}(A_i)$ such that

$$\|A_i - A_i'\|_2 < \varepsilon_1 := \sqrt{L}\left(\sqrt{1 + \frac{\varepsilon}{2L}} - 1 \right)$$

and

$$\operatorname{rank}(A_i') \leqslant \left\lceil \frac{\ell^2}{\varepsilon_1^2} \right\rceil \leqslant \left\lceil \frac{18L\ell^2}{\varepsilon^2} \right\rceil$$

where we have used for the last inequality that

$$\sqrt{1+x} \leqslant 1 + \frac{x}{2} - \frac{x^2}{9} \quad \text{for all } 0 \leqslant x \leqslant \frac{1}{4}, \tag{2}$$

applied to $x = \frac{\varepsilon}{2L}$. We define $M' := \left(\operatorname{tr}\left(A'_i A'_j\right)\right)_{i,j=1}^n$ and show that M' is an $\varepsilon/2$-approximation of M. Indeed, for $i, j \in [n]$ we have

$$\begin{aligned} \left|\operatorname{tr}(A_i A_j) - \operatorname{tr}(A'_i A'_j)\right| &\leqslant \left|\operatorname{tr}((A_i - A'_i)A_j)\right| + \left|\operatorname{tr}\left(A'_i(A_j - A'_j)\right)\right| \\ &\leqslant \|A_i - A'_i\|_2 \cdot \|A_j\|_2 + \|A_j - A'_j\|_2 \cdot \|A'_i\|_2 \\ &\leqslant \|A_i - A'_i\|_2 \cdot \|A_j\|_2 + \|A_j - A'_j\|_2 \cdot \left(\|A'_i - A_i\|_2 + \|A_i\|_2\right) \\ &\leqslant 2\varepsilon_1\sqrt{L} + \varepsilon_1^2 = \varepsilon/2, \end{aligned} \tag{3}$$

where the first and third inequality follow from the triangle inequality and the second inequality is Cauchy-Schwarz. For the last inequality we have used $\|A_i\|_2 = \sqrt{M_{ii}} \leqslant \sqrt{L}$.

Replacing ε by 2ε and using Lemma 6 then establishes the first of the upper bounds. We now continue to prove the second upper bound. For each $i \in [n]$ let the eigendecomposition of A'_i be

$$A'_i = \sum_{k=1}^m \lambda_{k,i} u_{k,i} u_{k,i}^t,$$

where $m := \lceil \ell^2/\varepsilon_1^2 \rceil$, and consider the nm-point set of all (normalized) eigenvectors of all A'_i:

$$\bigcup_{i=1}^n \{u_{1,i}, \ldots, u_{m,i}\} \subseteq \mathbb{R}^d.$$

By applying Theorem 11 with

$$\varepsilon_2 := -\frac{1}{3} + \frac{1}{3}\sqrt{1 + \frac{\varepsilon}{2\ell^2}}$$

we find that for

$$r \leqslant \frac{(6\ell)^4 \log\left(n \left\lceil \frac{18L\ell^2}{\varepsilon^2} \right\rceil + 1\right)}{\varepsilon^2} \tag{4}$$

there is a linear map $Q : \mathbb{R}^d \to \mathbb{R}^r$ such that

$$\left|u_{k,i}^t u_{k',j} - u_{k,i}^t Q^t Q u_{k',j}\right| \leqslant \varepsilon_2 \left(2 - u_{k,i}^t u_{k',j}\right) \leqslant 3\varepsilon_2. \tag{5}$$

for all $i, j \in [n], k, k' \in [m]$. Note that for the inequality in (4) we have again used (2) with $x := \varepsilon/2\ell^2$.

Set $v_{k,i} := Q u_{k,i} \in \mathbb{R}^r$ for all $i \in [n]$ and $k \in [m]$. For each $i \in [n]$, define the new psd matrix

$$A''_i := \sum_{k=1}^m \lambda_{k,i} v_{k,i} v_{k,i}^t \in \mathcal{S}_+^r,$$

and the new cpsd matrix $M'' = \left(\operatorname{tr}\left(A_i'' A_j''\right)\right)_{i,j=1}^n \in \mathcal{CPSD}^n$, whose cpsd-rank is at most r. We finally check that M'' is an $\varepsilon/2$-approximation of M'. For all $i, j \in [n]$ we have

$$
\begin{aligned}
\left|\operatorname{tr}\left(A_i' A_j'\right) - \operatorname{tr}\left(A_i'' A_j''\right)\right| &\leqslant \sum_{k,k'=1}^{m} \lambda_{k,i}\lambda_{k',j} \left|\left(u_{k,i}^t u_{k',j}\right)^2 - \left(v_{k,i}^t v_{k',j}\right)^2\right| \\
&= \sum_{k,k'=1}^{m} \lambda_{k,i}\lambda_{k',j} \left|u_{k,i}^t u_{k',j} - v_{k,i}^t v_{k',j}\right| \left|u_{k,i}^t u_{k',j} + v_{k,i}^t v_{k',j}\right| \\
&\leqslant \sum_{k,k'=1}^{m} \lambda_{k,i}\lambda_{k',j} \left(6\varepsilon_2 + 9\varepsilon_2^2\right) \\
&= \left(6\varepsilon_2 + 9\varepsilon_2^2\right) \operatorname{tr}(A_i')\operatorname{tr}(A_j') \\
&\leqslant \left(6\varepsilon_2 + 9\varepsilon_2^2\right) \ell^2 = \varepsilon/2
\end{aligned}
\tag{6}
$$

where the first inequality follows from the triangle inequality, the second from (5) and the third inequality from $\operatorname{tr}(A_i') = \operatorname{tr}(A_i) \leqslant \ell$.

Altogether, the matrix $N := M''$ is an ε-approximation of M, whose cpsd-rank is small enough to verify the second upper bound. □

Remark 13. (i) Which of the bounds in the main theorem is better depends on our setup. For instance, if we fix ε and let n approach infinity, then the bound obtained by applying the Johnson-Lindenstrauss Lemma is significantly smaller than the other. On the other hand, for n fixed and ε getting smaller, the first bound will be better.

(ii) If $M = (\langle A_i, A_j\rangle)_{i,j=1}^n$ is a completely positive matrix, with diagonal matrices $A_1, \ldots, A_n \in \mathcal{S}_+^d$, then the first approximation procedure can be used to generate a completely positive approximation. Indeed applying the Approximate Carathéodory Theorem will return diagonal matrices A_i'. Hence, the approximation N is completely positive with

$$\text{cp-rank}(N) \leqslant n \left\lceil \frac{9L\ell^2}{2\varepsilon^2} \right\rceil .$$

(iii) Note that the number ℓ in Theorem 12 is a kind of hidden complexity measure of the cpsd-matrix M. What we get from M directly are the numbers $\operatorname{tr}\left(A_i^2\right) = M_{ii}$, for any Gram representation $A_1, \ldots, A_n \in \mathcal{S}_+^d$. The numbers $\operatorname{tr}(A_i)$ are not uniquely determined however, and they encode information about the eigenvalue distribution of the psd-matrices in a Gram representation. One could upper bound them in terms of the numbers $\operatorname{tr}\left(A_i^2\right) = M_{ii}$, but this would involve a constant depending on d in general, which we want to avoid. So one should not employ this upper bound, and understand the approximation to really depend on the hidden complexity of M, but not on its cpsd-rank. One instance where this works well is when M admits a Gram decomposition $A_1, \ldots, A_n$ with all nonzero eigenvalues of all A_i larger equal to 1. A special case is stated in the following corollary.

Corollary 14. *Let $M \in \mathcal{CPSD}^n$ with Gram representation consisting of orthogonal projections $P_1, \ldots, P_n \in \mathcal{S}_+^d$. Further set $L \coloneqq \max_i M_{ii}$. Then for all $0 < \varepsilon < \frac{1}{2}L^2$ there exists some $N \in \mathcal{CPSD}^n$ with*

$$\textit{cpsd-rank}(N) \leqslant \min\left\{ n\left\lceil \frac{9L^3}{2\varepsilon^2} \right\rceil, \frac{(6L)^4 \log\left(n\left\lceil \frac{18L^3}{\varepsilon^2}\right\rceil + 1\right)}{\varepsilon^2} \right\}$$

and

$$|M_{ij} - N_{ij}| < \varepsilon \quad \textit{for all } i,j \in [n].$$

Proof. This is immediate from Theorem 12, since for orthogonal projections we have $\operatorname{tr}(P_i) = \operatorname{tr}\left(P_i^2\right) = M_{ii}$, and thus $L = \ell$. ☐

Example 15. Consider the identity matrix $I_n \in \mathcal{CPSD}^n$. A Gram representation is given by the elementary matrices $A_i \coloneqq E_{ii} \in \mathcal{S}_+^n$, and it is not hard to check that there is no Gram representation of smaller size, i.e. cpsd-rank$(I_n) = n$. The given A_i are rank one projections, so we have $\ell = \max_i \operatorname{tr}(A_i) = 1 = L$ for the given representation. The first upper bound from Theorem 12/Corollary 14 is not meaningful here, but the second is

$$\frac{6^4 \log\left(n\left\lceil \frac{18}{\varepsilon^2}\right\rceil + 1\right)}{\varepsilon^2},$$

which is smaller than n for fixed ε and large enough n. For example, for $\varepsilon = 1/2$ this happens at around $n = 8 \times 10^4$, for $\varepsilon = 1/10$ at around $n = 2.9 \times 10^6$.

Example 16. (i) Let $M \in \mathcal{CP}^n$ be a completely positive matrix. If we assume all diagonal entries of M to be one, this means M has a Gram representation by nonnegative unit vectors $v_1, \ldots, v_n$ (of some dimension). If we further understand these nonnegative vectors as diagonals of psd-matrices, we obtain a cpsd-decomposition of M for which the constant ℓ from Theorem 12 is precisely the maximum over all 1-norms of the v_i. The first upper bound for the approximation thus becomes

$$n\left\lceil \frac{9\max_i \|v_i\|_1^2}{2\varepsilon^2} \right\rceil$$

which, depending on the v_i, might be much smaller than the only known upper bound to the cp/cpsd-rank so far, which is the actual cp-rank of M and bounded by $\binom{n+1}{2} - 4$ (see [15]). Note again that the resulting approximation will again be completely positive, as explained in Remark 13 (ii).

(ii) Let $a, b, c, d \in \mathbb{R}_+^n$ with strictly positive entries. Further, define $C \coloneqq \operatorname{diag}(c_1, \ldots, c_n) \in \mathcal{S}_+^n$ and $D \coloneqq \operatorname{diag}(d_1, \ldots, d_n) \in \mathcal{S}_+^n$. Then, by Proposition 2.1. in [14] the $n^2 \times 2n$ matrix

$$V = \left(b \otimes C \,\middle|\, D \otimes a\right)$$

generates a completely positive matrix $M = V^t V \in \mathcal{CP}^{2n}$ with cp-rank$(M) = n^2$.

Now for $q \in (0,1)$ set $c, d \coloneqq (1, 1, \ldots, 1)^t$, and $a, b \coloneqq (1-q) \cdot \left(1, q, q^2, q^3, \ldots, q^{n-1}\right)^t$. For the columns v_i of V it holds that

$$\|v_i\|_1 = (1-q) \cdot \sum_{k=0}^{n-1} q^k \leqslant 1.$$

Thus both ℓ and L from Theorem 12 are at most 1, and hence, by the observation in (i), there exists a completely positive matrix $N \in \mathcal{CP}^{2n}$, which is an ε-approximation of M, and fulfills

$$\text{cpsd-rank}(N) \leqslant \text{cp-rank}(N) \leqslant 2n \left\lceil \frac{9}{2\varepsilon^2} \right\rceil .$$

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