# Matrices with high completely positive semidefinite rank 

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#### Abstract

A real symmetric matrix $M$ is completely positive semidefinite if it admits a Gram representation by (Hermitian) positive semidefinite matrices of any size $d$. The smallest such $d$ is called the (complex) completely positive semidefinite rank of $M$, and it is an open question whether there exists an upper bound on this number as a function of the matrix size. We construct completely positive semidefinite matrices of size $4 k^{2}+2 k+2$ with complex completely positive semidefinite rank $2^{k}$ for any positive integer $k$. This shows that if such an upper bound exists, it has to be at least exponential in the matrix size. For this we exploit connections to quantum information theory and we construct extremal bipartite correlation matrices of large rank. We also exhibit a class of completely positive matrices with quadratic (in terms of the matrix size) completely positive rank, but with linear completely positive semidefinite rank, and we make a connection to the existence of Hadamard matrices.


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## 1. Introduction

A matrix is said to be completely positive semidefinite if it admits a Gram representation by (Hermitian) positive semidefinite matrices of any size. The $n \times n$ completely positive semidefinite matrices form a convex cone, called the completely positive semidefinite cone, which is denoted by $\mathcal{C} \mathcal{S}_{+}^{n}$.

The motivation for the study of the completely positive semidefinite cone is twofold. Firstly, the completely positive semidefinite cone $\mathcal{C} \mathcal{S}_{+}^{n}$ is a natural analog of the completely positive cone $\mathcal{C} \mathcal{P}^{n}$, which consists of the matrices admitting a factorization by nonnegative vectors. The cone $\mathcal{C} \mathcal{P}^{n}$ is well studied (see, for example, the monograph [1]), and, in particular, it can be used to model classical graph parameters. For instance, [8] shows how to model the stability number of a graph as a conic optimization problem over the completely positive cone. A second motivation lies in the connection to quantum information theory. Indeed, the cone $\mathcal{C} \mathcal{S}_{+}^{n}$ was introduced in [17] to model quantum graph parameters (including quantum stability numbers) as conic optimization problems, an approach extended in [24] for quantum graph homomorphisms and in [26] for quantum correlations.

In this paper we are interested in the size of the factors needed in Gram representations of matrices. This type of question is of interest for factorizations by nonnegative vectors as well as by (Hermitian) positive semidefinite matrices.

Throughout we use the following notation. For $X, Y \in \mathbb{C}^{d \times d}, X^{*}$ is the conjugate transpose and $\langle X, Y\rangle=\operatorname{Tr}\left(X^{*} Y\right)$ is the trace inner product. For vectors $u, v \in \mathbb{R}^{d}$, $\langle u, v\rangle=u^{T} v$ denotes their Euclidean inner product.

A matrix $M$ is said to be completely positive if there exist nonnegative vectors $v_{1}, \ldots, v_{n} \in \mathbb{R}_{+}^{d}$ such that $M_{i, j}=\left\langle v_{i}, v_{j}\right\rangle$ for all $i, j \in[n]$. We call such a set of vectors a Gram representation or factorization of $M$ by nonnegative vectors. The smallest $d$ for which these vectors exist is denoted by $\operatorname{cp}-\operatorname{rank}(M)$ and is called the completely positive rank of $M$.

Similarly, a matrix $M$ is called completely positive semidefinite if there exist (real symmetric or complex Hermitian) positive semidefinite $d \times d$ matrices $X_{1}, \ldots, X_{n}$ such that $M_{i, j}=\left\langle X_{i}, X_{j}\right\rangle$ for all $i, j \in[n]$. We call such a set of matrices a Gram representation or factorization of $M$ by (Hermitian) positive semidefinite matrices. The smallest $d$ for which there exists a Gram representation of $M$ by Hermitian positive semidefinite $d \times d$ matrices is denoted by cpsd-rank $\mathbb{C}_{\mathbb{C}}(M)$, and the smallest $d$ for which these matrices can be taken to be real is denoted by $\operatorname{cpsd}-\operatorname{rank}_{\mathbb{R}}(M)$. We call this the real/complex completely positive semidefinite rank of $M$. If a matrix has a factorization by Hermitian positive semidefinite matrices, then it also has a factorization by real positive semidefinite matrices. In fact, for every $M \in \mathcal{C} \mathcal{S}_{+}^{n}$, we have

$$
{\operatorname{cpsd}-\operatorname{rank}_{\mathbb{C}}(M) \leq \operatorname{cpsd}-\operatorname{rank}_{\mathbb{R}}(M) \leq 2 \operatorname{cpsd}-\operatorname{rank}_{\mathbb{C}}(M), ~}_{\text {( }}
$$

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