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 positive semidefinite matrices (of any size d). The smallest such d is called the 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 show 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.

1. Introduction

A matrix is said to be *completely positive semidefinite* if it admits a Gram representation by 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 we denote by $\mathcal{CS}_+^n$.

The motivation for the study of the completely positive semidefinite cone is twofold. Firstly, the completely positive semidefinite cone $\mathcal{CS}_+^n$ is a natural analog of the completely positive cone $\mathcal{CP}^n$, which consists of the matrices admitting a factorization by nonnegative vectors. The cone $\mathcal{CP}^n$ is well studied (see, for example, the monograph [1]), and, in particular, it can be used to model classical graph parameters. For instance, [12] 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 $\mathcal{CS}_+^n$ was introduced in [13] to model quantum graph parameters (including quantum stability numbers) as conic optimization problems, an approach extended in [17] for quantum graph homomorphisms and in [20] 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 positive semidefinite matrices.

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 $M_{i,j} = \langle v_i, v_j \rangle$ for all i and j, where $\langle v_i, v_j \rangle = v_i^{\mathsf{T}} v_j$ denotes the Euclidean inner product. The smallest d for which these vectors exist is denoted by cp-rank(M) and is called the *completely positive rank* of M. Similarly, a matrix M is called *completely positive semidefinite* if there exist positive semidefinite matrices $X_1, \ldots, X_n \in \mathcal{S}_+^d$ such that $M_{i,j} = \langle X_i, X_j \rangle$ for all i and j, where $\langle X_i, X_j \rangle = \mathrm{Tr}(X_i X_j)$ is the trace inner product. The smallest d for which these matrices exist is denoted by cpsd-rank(M), and this is called this the *completely positive semidefinite rank* of M. We call such a set of vectors (matrices) a *Gram representation* or *factorization* of M by nonnegative vectors (positive semidefinite

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matrices). By construction, we have the following inclusions

$$\mathcal{CP}^n \subseteq \mathcal{CS}_+^n \subseteq \mathcal{S}_+^n \cap \mathbb{R}_+^{n\times n}.$$

The three cones coincide for $n \leq 4$ (since doubly nonnegative matrices of size $n \leq 4$ are completely positive), but both inclusions are strict for $n \geq 5$ (see [13] for details).

By Carathéodory's theorem, the completely positive rank of a matrix in $\mathcal{CP}^n$ is at most $\binom{n+1}{2}$. In [19] the following stronger bound is given:

$$\text{cp-rank}(M) \leq \binom{n+1}{2} - 4 \quad \text{for} \quad M \in \mathcal{CP}^n \quad \text{and} \quad n \geq 5, \tag{1}$$

which is also not known to be tight. No upper bound is known for the completely positive semidefinite rank of matrices in $\mathcal{CS}_+^n$. It is not even known whether such a bound exists. A positive answer would have strong implications. It would imply that the cone $\mathcal{CS}_+^n$ is closed. This, in turn, would imply that the set of quantum correlations is closed, since it can be seen as a projection of an affine slice of the completely positive semidefinite cone (see [16, 20]). Whether the set of quantum correlations is closed is an open question in quantum information theory. In contrast, as an application of the upper bound (1), the completely positive cone $\mathcal{CP}^n$ is easily seen to be closed. A description of the closure of the completely positive semidefinite cone in terms of factorizations by positive elements in von Neumann algebras can be found in [4]. Such factorizations were used to show a separation between the closure of $\mathcal{CS}_+^n$ and the doubly nonnegative cone $\mathcal{S}_+^n \cap \mathbb{R}_+^{n\times n}$ (see [9, 13]).

In this paper we show that if an upper bound exists for the completely positive semidefinite rank of matrices in $\mathcal{CS}_+^n$ then it needs to grow at least exponentially in the matrix size n. Our main result is the following:

Theorem 1.1. *For each positive integer r, there exists a completely positive semidefinite matrix M of size $r^2 + r + 2$ with* cpsd-rank$(M) \geq \sqrt{2}^{\lfloor r/2 \rfloor}$.

The proof of this result relies on a connection with quantum information theory and geometric properties of (bipartite) correlation matrices. We refer to the main text for the definitions of quantum and bipartite correlations. A first basic ingredient is the fact from [20] that a quantum correlation p can be realized in local dimension d if and only if there exists a certain completely positive semidefinite matrix with cpsd-rank at most d. Then, the key idea is to construct a class of quantum correlations p that need large local dimension. We construct such quantum correlations from bipartite correlation matrices. For this we use classical results of Tsirelson [21, 22], which characterize bipartite correlation matrices in terms of operator representations and provide a link to Clifford algebras. In this way we reduce the problem to the problem of finding bipartite correlation matrices that are extreme points of the set of bipartite correlations and have large rank. Interestingly, for our construction we use and combine classical results of Tsirelson with recent results in rigidity theory.

For the completely positive rank we have the quadratic upper bound (1), and completely positive matrices have been constructed whose completely positive rank grows quadratically in the size of the matrix. This is the case, for instance, for the matrices

$$M_k = \begin{pmatrix} I_k & \frac{1}{k}J_k \\ \frac{1}{k}J_k & I_k \end{pmatrix} \in \mathcal{CP}^{2k},$$

where cp-rank$(M_k) = k^2$. Here $I_k \in \mathcal{S}^k$ is the identity matrix and $J_k \in \mathcal{S}^k$ is the all-ones matrix. This leads to the natural question of how fast cpsd-rank(M_k) grows. As a second result we show that the completely positive semidefinite rank grows linearly for the matrices M_k, and we exhibit a link to the question of existence of Hadamard matrices. More precisely, we show that

$$k \leq \text{cpsd-rank}(M_k) \leq 2k,$$

with equality $\text{cpsd-rank}(M_k) = k$ if and only if there exists a real Hadamard matrix of order k.

The completely positive and completely positive semidefinite rank are symmetric analogs of the nonnegative and positive semidefinite rank. Here the nonnegative rank, denoted $\text{rank}_+(M)$, of a matrix $M \in \mathbb{R}_+^{m\times n}$, is the smallest integer d for which there exist nonnegative vectors $u_1,\ldots,u_m,v_1,\ldots,v_n \in \mathbb{R}_+^d$ such that $M_{i,j} = \langle u_i, v_j\rangle$ for all i and j, and the positive semidefinite rank, denoted $\text{rank}_{\text{psd}}(M)$, is the smallest d for which there exist positive semidefinite matrices $X_1,\ldots,X_m,Y_1,\ldots,Y_n \in \mathcal{S}_+^d$ such that $M_{i,j} = \langle x_i, y_j\rangle$ for all i and j. These notions have many applications, in particular to communication complexity and for the study of efficient linear or semidefinite extensions of convex polyhedra (see [25, 10]). Unlike in the symmetric setting, in the asymmetric setting the following bounds, which show a linear regime, can easily be checked:

$$\text{rank}_{\text{psd}}(A) \leq \text{rank}_+(A) \leq \min(m,n).$$

We refer to [8] and the references therein for a recent overview of results about the positive semidefinite rank.

Organization of the paper. In Section 2 we first present some simple properties of the completely positive semidefinite rank, and then investigate its value for the matrices M_k, where we also show a link to the existence of Hadamard matrices. We also give a simple heuristic for finding approximate positive semidefinite factorizations. The proof of our main result in Theorem 1.1 boils down to several key ingredients which we treat in the subsequent sections.

In Section 3 we group old and new results about the set of bipartite correlation matrices. In particular, we give a geometric characterization of the extreme points, we revisit some conditions due to Tsirelson and links to rigidity theory, and we construct a class of extreme bipartite correlations with optimal parameters.

In Section 4 we recall some characterizations, due to Tsirelson, of bipartite correlations in terms of operator representations. We also recall connections to Clifford algebras, and for bipartite correlations that are extreme points we relate their rank to the dimension of their operator representations.

Finally in Section 5 we introduce quantum correlations and recall their link to completely positive semidefinite matrices. We show how to construct quantum correlations from bipartite correlation matrices, and we prove the main theorem.

Note. Upon completion of this paper we learned of the recent independent work [18], where a class of matrices with exponential cpsd-rank is also constructed. The key idea of using extremal bipartite correlation matrices having large rank is the same. Our construction uses bipartite correlation matrices with optimized parameters meeting Tsirelson's upper bound (see Corollary 3.10). As a consequence, our completely positive semidefinite matrices have the best ratio between cpsd-rank and size that can be obtained using this technique.

2. Some properties of the completely positive semidefinite rank

In this section we consider the completely positive semidefinite rank of matrices in the completely positive cone. In particular, for a class of matrices, we show a quadratic separation in terms of the matrix size between both ranks. We also mention a simple heuristic for building completely positive semidefinite factorizations, which we have used to test several explicit examples.

We start by collecting some simple properties of the completely positive semidefinite rank. A first observation is that if a matrix M admits a Gram representation by Hermitian positive semidefinite matrices of size d, then it also admits a Gram representation by real symmetric positive semidefinite matrices of size $2d$, and thus M is completely positive semidefinite with $\text{cpsd-rank}(M) \leq 2d$. This is based on the well-known fact that mapping a Hermitian $d \times d$ matrix X to

$$\frac{1}{\sqrt{2}} \begin{pmatrix} \text{Re}(X) & -\text{Im}(X) \\ \text{Im}(X)^{\mathsf{T}} & \text{Re}(X) \end{pmatrix} \in \mathcal{S}^{2d}$$

is an isometry that preserves positive semidefiniteness. The completely positive semidefinite rank is subadditive, that is, for $A, B \in \mathcal{CS}_+^n$ we have

$$\text{cpsd-rank}(A + B) \leq \text{cpsd-rank}(A) + \text{cpsd-rank}(B),$$

which can be seen as follows: If A is the Gram matrix of $X_1, \dots, X_n \in \mathcal{S}_+^k$ and B is the Gram matrix of $Y_1, \dots, Y_n \in \mathcal{S}_+^r$, then $A + B$ is the Gram matrix of the matrices $X_1 \oplus Y_1, \dots, X_n \oplus Y_n \in \mathcal{S}_+^{k+r}$.

For $M \in \mathcal{CS}_+^n$ with $r = \text{cpsd-rank}(M)$, we have the inequality

$$\binom{r+1}{2} \geq \text{rank}(M),$$

since the factors of M in $\mathcal{S}_+^r$ yield another factorization of M by vectors in $\mathbb{R}^{\binom{r+1}{2}}$.

Finally, the next lemma shows that if the completely positive semidefinite rank of a matrix is high, then each factorization by positive semidefinite matrices must contain at least one matrix with high rank.

Lemma 2.1. *If $M \in \mathbb{R}^{n \times n}$ has a Gram representation by positive semidefinite matrices $X_1, \dots, X_n$ with* $\text{rank}(X_i) = r_i$*, then* $\text{cpsd-rank}(M) \leq r_1 + \ldots + r_n$.

Proof. Let $X_1, \dots, X_n \in \mathcal{S}_+^d$ be a Gram representation of M with $\text{rank}(X_i) = r_i$ for all $i \in [n]$. Let $k = r_1 + \ldots + r_n$. If $d > k$, then there exist orthonormal vectors $v_1, \dots, v_{d-k} \in \mathbb{R}^d$ such that $X_i v_j = 0$ for all i and j. Let $u_1, \dots, u_k$ be an orthonormal basis of $\text{span}\{v_1, \dots, v_{d-k}\}^\perp$, and let U be the matrix whose ith column is u_i. With $Y_i = U^* X_i U$ we have $\langle X_i, X_j \rangle = \langle Y_i, Y_j \rangle$ for all i and j, so $M = \text{Gram}(Y_1, \dots, Y_n)$. And since $Y_i \in \mathcal{S}_+^k$ for all i, this completes the proof. □

2.1. **A connection to the existence of Hadamard matrices.** Consider the $2k \times 2k$ matrix

$$M_k = \begin{pmatrix} I_k & \frac{1}{k} J_k \\ \frac{1}{k} J_k & I_k \end{pmatrix},$$

where I_k is the $k \times k$ identity matrix and J_k the $k \times k$ all-ones matrix. The completely positive rank of M_k equals k^2, which is well known and easy to check (see Proposition 2.2 below). The Drew-Johnson-Loewy (DJL) conjecture in [6] states that $\lfloor n^2/4 \rfloor$ is an upper bound on the completely positive rank of $n \times n$ matrices. Thus, for the matrices M_k, the completely positive rank attains this upper bound. The DJL conjecture holds for $n \leq 5$, but it was recently disproved in [3], where explicit matrices are constructed of size $7 \leq n \leq 11$ that have completely positive rank larger than the conjectured bound. For $k \geq 6$ the matrices M_k still have the largest known completely positive rank.

It is therefore natural to ask whether the matrices M_k also have large (quadratic in k) completely positive semidefinite rank. As we see below this is not the case. We show that the completely positive semidefinite rank is at most $2k$. We moreover show that it is equal to k if and only if a real Hadamard matrix of order k

exists, which suggests that determining the completely positive semidefinite rank is a difficult problem in general. A real *Hadamard* matrix of order k is a matrix $H \in \{\pm 1\}^{k\times k}$ with pairwise orthogonal columns. We use the following notation: The support of a vector $u \in \mathbb{R}^d$ is the set of indices $i \in [d]$ such that $u_i \neq 0$.

For completeness we first give a proof that the completely positive rank is k^2.

Proposition 2.2. *The completely positive rank of M_k is equal to k^2.*

Proof. For $i \in [k]$ consider the vectors $v_i = 1/\sqrt{k}\, e_i \otimes \mathbf{1}$ and $u_i = 1/\sqrt{k}\, \mathbf{1} \otimes e_i$, where e_i is the ith basis vector in $\mathbb{R}^k$ and $\mathbf{1}$ is the all-ones vector in $\mathbb{R}^k$. The vectors $v_1, \ldots, v_k, u_1, \ldots, u_k$ are nonnegative and form a Gram representation of M_k, which shows $\text{cp-rank}(M_k) \leq k^2$.

Suppose $M_k = \text{Gram}(v_1, v_2, \ldots, v_k, u_1, u_2, \ldots, u_k)$ with $v_i, u_i \in \mathbb{R}^d_+$. In the remainder of the proof we show $d \geq k^2$. We have $(M_k)_{i,j} = \delta_{ij}$ for $1 \leq i, j \leq k$. Since the vectors v_i are nonnegative, they must have disjoint supports. The same holds for the vectors $u_1, \ldots, u_k$. Since $(M_k)_{i,j} = 1/k > 0$ for $1 \leq i \leq k$ and $k+1 \leq j \leq 2k$, the support of v_i overlaps with the support of u_j for each i and j. This means that for each $i \in [k]$, the size of the support of the vector v_i is at least k. This is only possible if $d \geq k^2$. □

Proposition 2.3. *For each k we have $k \leq \text{cpsd-rank}(M_k) \leq 2k$, with equality $\text{cpsd-rank}(M_k) = k$ if and only if there exists a real Hadamard matrix of order k.*

Proof. Since $\text{cpsd-rank}(I_k) = k$, the lower bound $\text{cpsd-rank}(M_k) \geq k$ follows because I_k is a principal submatrix of M_k. We show the upper bound by giving an explicit factorization using real positive semidefinite $2k \times 2k$ matrices. For this we first give a factorization with Hermitian positive semidefinite $k \times k$ matrices. Let H_k be a complex Hadamard matrix of size k; that is, its entries are complex numbers with modulus one and its columns are pairwise orthogonal. Such a matrix exists for every k. Take for example

$$(H_k)_{i,j} = e^{2\pi \mathbf{i}(i-1)(j-1)/k} \quad \text{for} \quad i, j \in [k].$$

We define the factors

$$X_i = e_i e_i^{\mathsf{T}} \quad \text{and} \quad Y_i = \frac{u_i u_i^*}{k} \quad \text{for} \quad i \in [k],$$

where e_i is the ith standard basis vector of $\mathbb{R}^k$ and u_i is the ith column of H_k. By direct computation it follows that $M_k = \text{Gram}(X_1, \ldots, X_k, Y_1, \ldots, Y_k)$. As observed earlier from the Hermitian positive semidefinite matrices X_i, Y_i we can construct real positive semidefinite matrices of size $2k$ forming a Gram factorization of M_k. This shows $\text{cpsd-rank}(M_k) \leq 2k$.

We now show that $\text{cpsd-rank}(M_k) = k$ if and only if there exists a real Hadamard matrix of order k. One direction follows directly from the above proof: If a real Hadamard matrix of size k exists, then we can replace H_k by this real matrix and this yields a factorization by real positive semidefinite $k \times k$ matrices.

Conversely, assume that $\text{cpsd-rank}(M_k) = k$ and let $X_1, \ldots, X_k, Y_1, \ldots, Y_k \in \mathcal{S}^k_+$ be a Gram representation of M. We first show there exist two orthonormal bases $u_1, \ldots, u_k$ and $v_1, \ldots, v_k$ of $\mathbb{R}^k$ such that $X_i = u_i u_i^{\mathsf{T}}$ and $Y_i = v_i v_i^{\mathsf{T}}$. For this we observe that $I = \text{Gram}(X_1, \ldots, X_k)$, which implies $X_i \neq 0$ and $X_i X_j = 0$ for all $i \neq j$. Hence, the range of X_j is contained in the kernel of X_i for all $i \neq j$. This means that the range of X_i is orthogonal to the range of X_j. We now have $\sum_{i=1}^k \dim(\text{range}(X_i)) \leq k$ and $\dim(\text{range}(X_i)) \geq 1$ for all i. From this it follows that $\text{rank}(X_i) = 1$ for all $i \in [k]$. This means there exist $u_1, \ldots, u_k \in \mathbb{R}^k$ such that $X_i = u_i u_i^{\mathsf{T}}$ for all i. From $I = \text{Gram}(X_1, \ldots, X_k)$ it follows that the vectors $u_1, \ldots, u_k$ form an orthonormal basis of $\mathbb{R}^k$. The same argument can be made for the matrices Y_i, thus $Y_i = v_i v_i^\mathsf{T}$ and the vectors $v_1, \ldots, v_k$ form an orthonormal basis of $\mathbb{R}^k$. Up to an orthogonal transformation we may assume that the first basis is the standard basis; that is, $u_i = e_i$ for $i \in [k]$. We then obtain

$$\frac{1}{k} = (M_k)_{i,j+k} = \langle e_i, v_j \rangle^2 = \big((v_j)_i\big)^2 \quad \text{for} \quad i, j \in [k],$$

hence $(v_j)_i = \pm 1/\sqrt{k}$. Therefore, the $k \times k$ matrix whose kth column is $\sqrt{k}\, v_k$ is a real Hadamard matrix. □

The above proposition leaves open the exact determination of cpsd-rank(M_k) for the cases where a real Hadamard matrix of order k does not exist. Extensive experimentation using the heuristic from Section 2.2 suggests that for $k = 3, 5, 6, 7$ the cpsd-rank of M_k equals $2k$, which leads to the following question:

Question 2.4. *Is the completely positive semidefinite rank of M_k equal to $2k$ if a real Hadamard matrix of size $k \times k$ does not exist?*

We also used the heuristic from Section 2.2 to check numerically that the aforementioned matrices from [3], which have completely positive rank greater than $\lfloor n^2/4 \rfloor$, have small (smaller than n) cpsd-rank. In fact, in our numerical experiments we never found a completely positive $n \times n$ matrix for which we could not find a factorization in dimension n, which leads to the following question:

Question 2.5. *Is the completely positive semidefinite rank of a completely positive $n \times n$ matrix upper bounded by n?*

2.2. **A heuristic for finding Gram representations.** In this section we give an adaptation to the symmetric setting of the seesaw method from [24], which is used to find good quantum strategies for nonlocal games. Given a matrix $M \in \mathcal{CS}_+^n$ with cpsd-rank$(M) \leq d$, we give a heuristic to find a Gram representation of M by positive semidefinite $d \times d$ matrices. Although this heuristic is not guaranteed to converge to a factorization of M, for small n and d (say, $n, d \leq 10$) it works well in practice by restarting the algorithm several times. The following algorithm seeks to minimize the function

$$E(X_1, \ldots, X_n) = \|\mathrm{Gram}(X_1, \ldots, X_n) - M\|_\infty.$$

Algorithm 2.6. *Initialize the algorithm by setting $k = 1$ and generating random matrices $X_1^0, \ldots, X_n^0 \in \mathcal{S}_+^d$ that satisfy $\langle X_i^0, X_i^0 \rangle = M_{i,i}$ for all $i \in [n]$. Iterate the following steps:*

(1) *Let $(\delta, Y_1, \ldots, Y_n)$ be a (near) optimal solution of the semidefinite program*
$$\min\Big\{\delta : \delta \in \mathbb{R}_+,\, Y_1, \ldots, Y_n \in \mathcal{S}_+^d,\, \Big|\big\langle X_i^{k-1}, Y_j \big\rangle - M_{i,j}\Big| \leq \delta \text{ for } i, j \in [n]\Big\}.$$
(2) *Perform a line search to find the scalar $r \in [0, 1]$ minimizing*
$$E\big((1-r)X_1^{k-1} + rY_1, \ldots, (1-r)X_n^{k-1} + rY_n\big),$$
and set $X_i^k = (1-r)X_i^{k-1} + rY_i$ for each $i \in [n]$.
(3) *If $E(X_1^k, \ldots, X_n^k)$ is not small enough, increase k by one and go to step (1). Otherwise, return the matrices X_1^k, …, X_n^k.*

3. The set of bipartite correlations

In this section we define the set $\mathrm{Cor}(m, n)$ of bipartite correlations and we discuss properties of the extreme points of $\mathrm{Cor}(m, n)$, which will play a crucial role in the construction of $\mathcal{CS}_+$-matrices with large cpsd-rank. In particular we give a characterization of the extreme points of $\mathrm{Cor}(m, n)$ in terms of extreme points of the related set $\mathcal{E}_{m+n}$ of correlation matrices. We use it to give a simple construction of a class of extreme points of $\mathrm{Cor}(m, n)$ with rank r, when $m = n = \binom{r+1}{2}$. We also revisit conditions for extreme points introduced by Tsirelson [21] and point out links with universal rigidity. Based on these we can construct extreme points of $\mathrm{Cor}(m, n)$ with rank r when $m = r$ and $n = \binom{r}{2} + 1$, which are used to prove our main result (Theorem 1.1).

A matrix $C \in \mathbb{R}^{m\times n}$ is called a *bipartite correlation matrix* if there exist real unit vectors $x_1, \dots, x_m, y_1, \dots, y_n \in \mathbb{R}^d$ (for some $d \geq 1$) such that $C_{s,t} = \langle x_s, y_t\rangle$ for all $s \in [m]$ and $t \in [n]$. Following Tsirelson [21], any such system of real unit vectors is called a *C-system*. We let $\mathrm{Cor}(m, n)$ denote the set of all $m \times n$ bipartite correlation matrices.

The *elliptope* $\mathcal{E}_n$ is defined as

$$\mathcal{E}_n = \Big\{E \in \mathcal{S}^n_+ : E_{ii} = 1 \text{ for } i = 1, \dots, n\Big\},$$

its elements are the *correlation matrices*, which can alternatively be defined as all matrices of the form $(\langle z_i, z_j\rangle)^n_{i,j=1}$ for some real unit vectors $z_1, \dots, z_n \in \mathbb{R}^d$ $(d \geq 1)$. We have the surjective projection

$$\pi\colon \mathcal{E}_{m+n} \to \mathrm{Cor}(m, n), \begin{pmatrix} Q & C \\ C^{\mathsf{T}} & R \end{pmatrix} \mapsto C. \tag{2}$$

Hence, $\mathrm{Cor}(m, n)$ is a projection of the elliptope $\mathcal{E}_{m+n}$ and therefore a convex set. Given $C \in \mathrm{Cor}(m, n)$, any matrix $E \in \mathcal{E}_{m+n}$ such that $\pi(E) = C$ is called an *extension* of C to the elliptope and we let $\mathrm{fib}(C)$ denote the fiber (the set of extensions) of C.

Theorem 3.3 below characterizes extreme points of $\mathrm{Cor}(m, n)$ in terms of extreme points of $\mathcal{E}_{m+n}$. It is based on two intermediary results. The first result relates extreme points $C \in \mathrm{Cor}(m, n)$ to properties of their set of extensions $\mathrm{fib}(C)$. It is shown in [7] (in a more general setting); we omit the (easy) proof.

Lemma 3.1 ([7, Lemma 2.4])**.** *Let $C \in \mathrm{Cor}(m, n)$. Then C is an extreme point of $\mathrm{Cor}(m, n)$ if and only if the set $\mathrm{fib}(C)$ is a face of $\mathcal{E}_{m+n}$. Moreover, if C is an extreme point of $\mathrm{Cor}(m, n)$, then every extreme point of $\mathrm{fib}(C)$ is an extreme point of $\mathcal{E}_{m+n}$.*

The second result (from Tsirelson [21]) shows that every extreme point C of $\mathrm{Cor}(m, n)$ has a unique extension E in $\mathcal{E}_{m+n}$, we give a proof for completeness.

Lemma 3.2 ([21])**.** *Assume C is an extreme point of $\mathrm{Cor}(m, n)$.*

(i) *If $x_1, \dots, x_m, y_1, \dots, y_n$ is a C-system, then*

$$\mathrm{Span}\{x_1, \dots, x_m\} = \mathrm{Span}\{y_1, \dots, y_n\}.$$

(ii) *The matrix C has a unique extension to a matrix $E \in \mathcal{E}_{m+n}$, and there exists a C-system $x_1, \dots, x_m, y_1, \dots, y_n \in \mathbb{R}^r$, with $r = \mathrm{rank}(C)$, such that*

$$E = \mathrm{Gram}(x_1, \dots, x_m, y_1, \dots, y_n).$$

Proof. We will use the following observation: Each matrix $C = (\langle a_s, b_t\rangle)_{s\in[m],t\in[n]}$, where a_s, b_t are vectors with $\|a_s\|, \|b_t\| \leq 1$, belongs to $\mathrm{Cor}(m, n)$ since it satisfies

$$C_{s,t} = \left\langle \begin{pmatrix} a_s \\ \sqrt{1 - \|a_s\|^2} \\ 0 \end{pmatrix}, \begin{pmatrix} b_t \\ 0 \\ \sqrt{1 - \|b_t\|^2} \end{pmatrix} \right\rangle \quad \text{for all } (s, t) \in [m] \times [n].$$

(i) Set $V = \mathrm{Span}\{x_1, \dots, x_m\}$ and assume $y_k \notin V$ for some $k \in [n]$. Let w denote the orthogonal projection of y_k onto V. Then $\|w\| < 1$ and one can choose a nonzero vector $u \in V$ such that $\|w \pm u\| \leq 1$. Define the matrices $C^{\pm} \in \mathbb{R}^{m\times n}$ by

$$C^{\pm}_{s,t} = \begin{cases} \langle x_s, w \pm u\rangle & \text{if } t = k, \\ \langle x_s, y_t\rangle & \text{if } t \neq k. \end{cases}$$

Then, $C^{\pm} \in \mathrm{Cor}(m,n)$ (by the above observation) and $C = (C^+ + C^-)/2$. As C is an extreme point of $\mathrm{Cor}(m,n)$ one must have $C = C^+ = C^-$. Hence u is orthogonal to each x_s and thus $u = 0$, a contradiction. This shows the inclusion $\mathrm{Span}\{y_1, \ldots, y_m\} \subseteq \mathrm{Span}\{x_1, \ldots, x_m\}$ and the reverse one follows in the same way.

(ii) Assume $\{x'_s, y'_t\}$ and $\{x''_s, y''_t\}$ are two C-systems. We show $\langle x'_r, x'_s\rangle = \langle x''_r, x''_s\rangle$ for all $r, s \in S$ and $\langle y'_t, y'_u\rangle = \langle y''_t, y''_u\rangle$ for all $t, u \in T$. For this define the vectors $x_s = (x'_s \oplus x''_s)/\sqrt{2}$ and $y_t = (y'_t \oplus y''_t)/\sqrt{2}$, which again form a C-system. Using (i), for any $s \in S$, there exist scalars λ^s_t such that $x_s = \sum_{t\in T} \lambda^s_t y_t$ and thus $x'_s = \sum_{t\in T} \lambda^s_t y'_t$ and $x''_s = \sum_{t\in T} \lambda^s_t y''_t$. This shows

$$\langle x'_r, x'_s\rangle = \sum_{t\in T} \lambda^r_t \langle y'_t, x'_s\rangle = \sum_{t\in T} \lambda^r_t C_{s,t} = \sum_{t\in T} \lambda^r_t \langle y''_t, x''_s\rangle = \langle x''_r, x''_s\rangle$$

for all $r, s \in S$. The analogous argument shows $\langle y'_t, y'_u\rangle = \langle y''_t, y''_u\rangle$ for all $t, u \in T$. This shows C has a unique extension to a matrix $E \in \mathcal{E}_{m+n}$.

Finally, we show that $\mathrm{rank}(E) = \mathrm{rank}(C)$. Say E is the Gram matrix of $x_1, \ldots, x_m, y_1, \ldots, y_n$. In view of (i), $\mathrm{rank}(E) = \mathrm{rank}\{x_1, \ldots, x_m\}$ and thus it suffices to show that $\mathrm{rank}\{x_1, \ldots, x_m\} \le \mathrm{rank}(C)$. For this note that if $\{x_s : s \in I\}$ (for some $I \subseteq S$) is linearly independent then the corresponding rows of C are linearly independent, since $\sum_{s\in I} \lambda_s \langle x_s, y_t\rangle = 0$ (for all $t \in T$) implies $\sum_{s\in I} \lambda_s x_s = 0$ (using (i)) and thus $\lambda_s = 0$ for all s. □

Theorem 3.3. *A matrix C is an extreme point of* $\mathrm{Cor}(m,n)$ *if and only if C has a unique extension to a matrix $E \in \mathcal{E}_{m+n}$ and E is an extreme point of $\mathcal{E}_{m+n}$.*

Proof. Direct application of Lemma 3.1 and Lemma 3.2 (ii). □

We can use the following lemma to construct explicit examples of extreme points of $\mathrm{Cor}(m,n)$ for the case $m = n$.

Lemma 3.4. *Each extreme point of $\mathcal{E}_n$ is an extreme point of* $\mathrm{Cor}(n,n)$.

Proof. Let C be an extreme point of $\mathcal{E}_n$. Define the matrix

$$E = \begin{pmatrix} C & C \\ C & C \end{pmatrix}.$$

Then $E \in \mathcal{E}_{2n}$ is an extension of C. In view of Theorem 3.3 it suffices to show that E is the unique extension of C and that E is an extreme point of $\mathcal{E}_{2n}$. With $e_1, \ldots, e_n$ denoting the standard unit vectors in $\mathbb{R}^n$, observe that the vectors $e_i \oplus -e_i$ ($i \in [n]$) lie in the kernel of any matrix $E' \in \mathrm{fib}(C)$, since E' and C have an all-ones diagonal. This implies that $\mathrm{fib}(C) = \{E\}$. We now show that E is an extreme point of $\mathcal{E}_{2n}$. For this let $E_1, E_2 \in \mathcal{E}_{2n}$ and $0 < \lambda < 1$ such that $E = \lambda E_1 + (1-\lambda)E_2$. As the kernel of E is the intersection of the kernels of E_1 and E_2, the vectors $e_i \oplus -e_i$ belong to the kernel of E_1 and E_2 and thus

$$E_1 = \begin{pmatrix} C_1 & C_1 \\ C_1 & C_1 \end{pmatrix} \quad \text{and} \quad E_2 = \begin{pmatrix} C_2 & C_2 \\ C_2 & C_2 \end{pmatrix}$$

for some $C_1, C_2 \in \mathcal{E}_n$. Hence, $C = \lambda C_1 + (1-\lambda)C_2$, which implies $C = C_1 = C_2$, since C is an extreme point of $\mathcal{E}_n$. Thus $E = E_1 = E_2$, which completes the proof. □

The above lemma shows how to construct extreme points of $\mathrm{Cor}(n,n)$ from extreme points of the elliptope $\mathcal{E}_n$. Li and Tam [15] give the following characterization of the extreme points of $\mathcal{E}_n$.

Theorem 3.5 ([15])**.** *Consider a matrix $E \in \mathcal{E}_n$ with rank r and unit vectors $z_1, \ldots, z_n \in \mathbb{R}^r$ such that $E = \mathrm{Gram}(z_1, \ldots, z_n)$. Then E is an extreme point of $\mathcal{E}_n$ if and only if*

$$\binom{r+1}{2} = \dim(\mathrm{Span}\{z_1 z_1^\mathsf{T}, \ldots, z_n z_n^\mathsf{T}\}). \tag{3}$$

In particular, if E is an extreme point of $\mathcal{E}_n$, then $\binom{r+1}{2} \leq n$.

Example 3.6 ([15])**.** *For each integer $r \geq 1$ there exists an extreme point of $\mathcal{E}_n$ of rank r, where $n = \binom{r+1}{2}$. For example, let $e_1, \ldots, e_r$ be the standard basis vectors of $\mathbb{R}^r$ and define*

$$E = \mathrm{Gram}\Big(e_1, \ldots, e_r, \frac{e_1 + e_2}{\sqrt{2}}, \frac{e_1 + e_3}{\sqrt{2}}, \ldots, \frac{e_{r-1} + e_r}{\sqrt{2}}\Big).$$

Then E is an extreme point of $\mathcal{E}_n$ of rank r.

Note that the above example is optimal in the sense that a rank r extreme point of $\mathcal{E}_n$ can exist only if $n \geq \binom{r+1}{2}$ (by Theorem 3.5). By combining this with Lemma 3.4, this gives a class of extreme points of $\mathrm{Cor}(m,n)$ with rank r and $m = n = \binom{r+1}{2}$.

If C is an extreme point of $\mathrm{Cor}(m,n)$ with rank r, then by Theorems 3.3 and 3.5 we have $\binom{r+1}{2} \leq m+n$. Tsirelson [21] claimed the stronger bound $\binom{r+1}{2} \leq m+n-1$ (see Corollary 3.10 below). In what follows we will construct extreme points of $C(m,n)$ with rank r and $m = r$, $n = \binom{r}{2} + 1$, thus with optimal parameters with respect to Tsirelson's upper bound.

For this we need to investigate in more detail the unique extension property of extreme points of $\mathrm{Cor}(m,n)$. Let $C \in \mathrm{Cor}(m,n)$ with rank r, let $\{x_s\}$, $\{y_t\}$ be a C-system in $\mathbb{R}^r$, and let $E = \mathrm{Gram}(x_1, \ldots, x_m, y_1, \ldots, y_n) \in \mathcal{E}_{m+n}$. In view of Theorem 3.3, if C is an extreme point of $\mathrm{Cor}(m,n)$, then E is the unique extension of C in $\mathcal{E}_{m+n}$. This uniqueness property can be rephrased as the requirement that an associated semidefinite program has a unique solution. Namely, consider the following dual pair of semidefinite programs:

$$\max\Big\{0 : X \in \mathcal{S}_+^{S\cup T},\ X_{k,k} = 1 \text{ for } k \in S \cup T,\ X_{s,t} = C_{s,t} \text{ for } s \in S, t \in T\Big\}, \tag{4}$$

$$\min\Big\{\sum_{s\in S}\lambda_s + \sum_{t\in T}\mu_t + 2\sum_{s\in S, t\in T} W_{s,t}C_{s,t} : \Omega = \begin{pmatrix} \mathrm{Diag}(\lambda) & W \\ W^\mathsf{T} & \mathrm{Diag}(\mu)\end{pmatrix} \in \mathcal{S}_+^{S\cup T}\Big\}. \tag{5}$$

The feasible region of problem (4) consists of all possible extensions of C in $\mathcal{E}_{m+n}$, and the feasible region of (5) consists of the positive semidefinite matrices Ω whose support (consisting of all off-diagonal pairs (i,j) with $\Omega_{i,j} \neq 0$) is contained in the complete bipartite graph $K_{m,n}$ corresponding to the bipartition $S \cup T$. Moreover, the optimal values of both problems are equal to 0, and for any primal feasible (optimal) X and dual optimal Ω the equality$X\Omega = 0$ holds, implying $\mathrm{rank}(X) + \mathrm{rank}(\Omega) \leq m + n$. The next result, shown in [14] in the more general context of universal rigidity, shows that equality $\mathrm{rank}(X) + \mathrm{rank}(\Omega) = m + n$ (also known as *strict complementarity*) implies that X is the *unique* feasible solution of program (4), and thus C has a *unique* extension in $\mathcal{E}_{m+n}$.

Theorem 3.7 ([14, Theorem 3.2])**.** *Let $C \in \mathrm{Cor}(m,n)$ and let $\{x_s\}$, $\{y_t\}$ be a C-system spanning $\mathbb{R}^r$. Assume $E = \mathrm{Gram}(x_1, \ldots, x_m, y_1, \ldots, y_n)$ is an extreme point of $\mathcal{E}_{m+n}$. If there exists an optimal solution Ω of program (5) with $\mathrm{rank}(\Omega) = m + n - r$, then E is the only extension of C in $\mathcal{E}_{m+n}$.*

In addition one can relate uniqueness of an extension of C in the elliptope to the existence of a quadric separating the two point sets $\{x_s\}$ and $\{y_t\}$ (Theorem 3.9 below). Roughly speaking, such a quadric allows us to construct a suitable optimal dual solution Ω and to apply Theorem 3.7. This property was stated by Tsirelson [21, 22], however without proof. Interestingly, an analogous result was shown recently by Connelly and Gortler [5] in the setting of universal rigidity. We will give a proof sketch of Theorem 3.9, based on Theorem 3.7, arguments in [5], and the following basic property of semidefinite programs (which can be seen as an analog of Farkas' lemma for linear programs).

Theorem 3.8. *Given $A_1, \dots, A_m \in \mathcal{S}^n$ and $b \in \mathbb{R}^m$, and assume that there exists a matrix $X \in \mathcal{S}^n$ such that $\langle A_j, X\rangle = b_j$ for all $j \in [m]$. Then exactly one of the following two alternatives holds:*

(i) *There exists a matrix $X \succ 0$ such that $\langle A_j, X\rangle = b_j$ for all $j \in [m]$.*
(ii) *There exists $y \in \mathbb{R}^m$ such that $\Omega = \sum_{j=1}^m y_j A_j \succeq 0$, $\Omega \neq 0$, and $\Omega X = 0$.*

Theorem 3.9 ([21, 22])**.** *Let $C \in \mathrm{Cor}(m, n)$, let $x_1, \dots, x_m, y_1, \dots, y_n \in \mathbb{R}^r$ be a C-system spanning $\mathbb{R}^r$, and let $E = \mathrm{Gram}(x_1, \dots, x_m, y_1, \dots, y_n) \in \mathcal{E}_{m+n}$.*

(i) *If C is an extreme point of $\mathrm{Cor}(m, n)$, then there exist nonnegative scalars $\lambda_1, \dots, \lambda_m$, $\mu_1, \dots, \mu_n$, not all equal to zero, such that*

$$\sum_{s=1}^m \lambda_s x_s x_s^{\mathsf{T}} = \sum_{t=1}^n \mu_t y_t y_t^{\mathsf{T}}. \tag{6}$$

(ii) *If E is an extreme point of $\mathcal{E}_{m+n}$ and there exist strictly positive scalars $\lambda_1, \dots, \lambda_m, \mu_1, \dots, \mu_n$ for which relation (6) holds, then C is an extreme point of $\mathrm{Cor}(m, n)$.*

Proof. (i) By assumption, C is an extreme point of $\mathrm{Cor}(m, n)$, so by Lemma 3.2 (ii) E is the only feasible solution of the program (4). As E has rank $r < m+n$, it follows that the program (4) does not have a positive definite feasible solution. Applying Theorem 3.8 it follows that there exists a nonzero matrix Ω that is feasible for the dual program (5) and satisfies $\Omega E = 0$. This gives:

$$\lambda_s x_s + \sum_{t\in T} W_{s,t} y_t = 0 \ (s \in S), \quad \mu_t y_t + \sum_{s\in S} W_{s,t} x_s = 0 \ (t \in T).$$

Since $\Omega \succeq 0$, the scalars λ_s, μ_t are nonnegative. We claim that they satisfy (6). We multiply the left relation by x_s^{T} and the right one by y_t^{T} to obtain

$$\lambda_s x_s x_s^{\mathsf{T}} + \sum_{t\in T} W_{s,t} y_t x_s^{\mathsf{T}} = 0 \ (s \in S), \quad \mu_t y_t y_t^{\mathsf{T}} + \sum_{s\in S} W_{s,t} x_s y_t^{\mathsf{T}} = 0 \ (t \in T).$$

Summing the left relation over $s \in S$ and the right one over $t \in T$ we get:

$$\sum_{s\in S} \lambda_s x_s x_s^{\mathsf{T}} = -\sum_{s\in S}\sum_{t\in T} W_{s,t} y_t x_s^{\mathsf{T}} = \sum_{t\in T} \mu_t y_t y_t^{\mathsf{T}},$$

and thus (6) holds.

(ii) Assume that E is an extreme point of $\mathcal{E}_{m+n}$ and that there exist strictly positive scalars $\lambda_1, \dots, \lambda_m, \mu_1, \dots, \mu_n$ for which (6) holds. The key idea is to construct a matrix Ω that is optimal for the program (5) and has rank $m + n - r$, since then we can apply Theorem 3.7 and conclude that E is the only extension of C in $\mathcal{E}_{m+n}$. The construction of such a matrix Ω is analogous to the construction given in [5] for frameworks (see Theorem 4.3 and its proof), so we omit the details. □

Corollary 3.10 ([22])**.** *If C is an extreme point of* $\mathrm{Cor}(m,n)$ *with* $\mathrm{rank}(C) = r$, *then*

$$\binom{r+1}{2} \leq n + m - 1. \tag{7}$$

Proof. Let $x_1, \ldots, x_m, y_1, \ldots, y_n \in \mathbb{R}^r$ be a C-system spanning $\mathbb{R}^r$ and E their Gram matrix. As E is an extreme point of $\mathcal{E}_{m+n}$, it follows from relation (3) that $\mathcal{S}^r$ is spanned by the $m+n$ matrices $x_i x_i^\mathsf{T}, y_j y_j^\mathsf{T}$ $(i \in S, j \in T)$. Combining this with the identity (6) this implies that $\mathcal{S}^r$ is spanned by a set of $m+n-1$ matrices and thus its dimension $\binom{r+1}{2}$ is at most $m+n-1$. □

We conclude with constructing a new family of extreme points C of $\mathrm{Cor}(m,n)$ with $\mathrm{rank}(C) = r$, $m = r$, and $n = \binom{r}{2} + 1$, thus showing that inequality (7) is tight. Such a family of bipartite correlation matrices can also be inferred from [23], where the correlation matrices are obtained through analytical methods as optimal solutions of linear optimization problems over $\mathrm{Cor}(m,n)$. Instead, we use the sufficient conditions for extremality of bipartite correlations given above.

We construct matrices $E, \Omega \in \mathcal{S}^{r+n}$ that satisfy the conditions of Theorem 3.7; that is, E is an extreme point of $\mathcal{E}_{r+n}$, Ω is positive semidefinite with support contained in the complete bipartite graph $K_{r,n}$, $\mathrm{rank}(E) = r$, $\mathrm{rank}(\Omega) = n - r$, and $E\Omega = 0$. Our construction of Ω is inspired by [11], which studies the maximum possible rank of extremal positive semidefinite matrices with a complete bipartite support.

Consider the matrix $B \in \mathbb{R}^{r \times n}$ whose last column is the all-ones vector and whose remaining $n - 1 = \binom{r}{2}$ columns are indexed by the pairs (i,j) with $1 \leq i < j \leq r$, with entries $B_{i,(i,j)} = 1$, $B_{j,(i,j)} = -1$ for $1 \leq i < j \leq r$, and all other entries 0. Note that $BB^\mathsf{T} = rI_r$. Then define the following matrices:

$$\Omega' = \begin{pmatrix} nI_r & \sqrt{n}B \\ \sqrt{n}B^\mathsf{T} & rI_n \end{pmatrix}, \quad E' = \begin{pmatrix} I_r & -\frac{\sqrt{n}}{r}B \\ -\frac{\sqrt{n}}{r}B^\mathsf{T} & \frac{n}{r^2}B^\mathsf{T}B \end{pmatrix} \in \mathcal{S}_{r+n}.$$

One can easily verify that $\Omega', E' \succeq 0$, $\Omega' E' = 0$, $\mathrm{rank}\,\Omega' = n$, and $\mathrm{rank}(E') = r$. It suffices now to modify the matrix E' in order to get a matrix E with an all-ones diagonal. For this, consider the diagonal matrix

$$D = I_r \oplus \frac{r}{\sqrt{2n}} I_{n-1} \oplus \sqrt{\frac{r}{n}} I_1$$

and set $E = DE'D$ and $\Omega = D^{-1}\Omega' D^{-1}$. Then E has an all-ones diagonal, it is in fact the Gram matrix of the vectors $e_1, \ldots, e_r$, $(e_i - e_j)/\sqrt{2}$ (for $1 \leq i < j \leq r$), and $(e_1 + \ldots + e_r)/\sqrt{r}$, and thus E is an extreme point of $\mathcal{E}_{r+n}$. Moreover, $\Omega E = 0$, $\mathrm{rank}\, E = r$, and $\mathrm{rank}\,\Omega = n$. Therefore the conditions of Theorem 3.7 are fulfilled and we can conclude that the matrix $C = \pi(E)$ is an extreme point of $\mathrm{Cor}(r,n)$. So we have shown the following result.

Lemma 3.11. *For each integer $r \geq 1$ and $n = \binom{r}{2} + 1$, there exists a matrix $C \in \mathrm{Cor}(r,n)$ that is an extreme point of $C(r,n)$ and has rank r. We can take C to be the matrix with columns $(e_i - e_j)/\sqrt{2}$ (for $1 \leq i < j \leq r$) and $(e_1 + \ldots + e_r)/\sqrt{r}$, where $e_1, \ldots, e_r \in \mathbb{R}^r$ is the standard basis.*

4. Lower bounding the size of operator representations

We start with recalling, in Theorem 4.1, some equivalent characterizations for bipartite correlations in terms of operator representations, due to Tsirelson. For this consider a matrix $C \in \mathbb{R}^{m \times n}$. We say that C admits a *tensor operator representation* if there exist an integer d (the *local dimension*), a unit vector $\psi \in \mathbb{C}^d \otimes \mathbb{C}^d$, and

Hermitian $d \times d$ matrices $\{X_s\}_{s=1}^m$ and $\{Y_t\}_{t=1}^n$ with spectra contained in $[-1,1]$, such that $C_{s,t} = \psi^*(X_s \otimes Y_t)\psi$ for all s and t.

Moreover we say that C admits a (finite dimensional) *commuting operator representation* if there exist an integer d, a Hermitian positive semidefinite $d \times d$ matrix W with $\mathrm{trace}(W) = 1$, and Hermitian $d \times d$ matrices $\{X_s\}$ and $\{Y_t\}$ with spectra contained in $[-1,1]$, such that $X_sY_t = Y_tX_s$ and $C_{s,t} = \mathrm{Tr}(X_sY_tW)$ for all s and t. A commuting operator representation is said to be *pure* if $\mathrm{rank}(W) = 1$.

Existence of these various operator representations relies on using Clifford algebras. For an integer $r \geq 1$ the *Clifford algebra* $\mathcal{C}(r)$ of order r can be defined as the universal C^*-algebra with Hermitian generators $a_1, \dots, a_r$ and relations

$$a_i^2 = 1 \quad \text{and} \quad a_ia_j + a_ja_i = 0 \quad \text{for} \quad i \neq j. \tag{8}$$

We call these relations the *Clifford relations.* To represent the elements of $\mathcal{C}(r)$ by matrices we can use the following map, which is a $*$-isomorphism onto its image:

$$\varphi_r\colon \mathcal{C}(r) \to \mathbb{C}^{2^{\lceil r/2\rceil} \times 2^{\lceil r/2\rceil}},\ \varphi_r(a_i) = \begin{cases} Z^{\otimes \frac{i-1}{2}} \otimes X \otimes I^{\otimes \lceil \frac{r}{2}\rceil - \frac{i+1}{2}} & \text{for } i \text{ odd},\\ Z^{\otimes \frac{i-2}{2}} \otimes Y \otimes I^{\otimes \lceil \frac{r}{2}\rceil - \frac{i}{2}} & \text{for } i \text{ even}.\end{cases} \tag{9}$$

Here we use the *Pauli matrices*

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For even r the representation φ_r is irreducible and thus $\mathcal{C}(r)$ is isomorphic to the full matrix algebra with matrix size $2^{\lceil r/2\rceil}$. For odd r the representation φ_r decomposes as a direct sum of two irreducible representations, each of dimension $2^{\lfloor r/2\rfloor}$. Therefore, if $X_1, \dots, X_r$ is a set of Hermitian matrices satisfying the relations $X_i^2 = I$ and $X_iX_j + X_jX_i = 0$ for $i \neq j$, then they must have size at least $2^{\lfloor r/2\rfloor}$.

Theorem 4.1 ([21])**.** *Let $C \in \mathbb{R}^{m\times n}$. The following statements are equivalent:*
1. *C is a bipartite correlation.*
2. *C admits a tensor operator representation.*
3. *C admits a pure commuting operator representation.*
4. *C admits a commuting operator representation.*

Proof. (1) $\Rightarrow$ (2) Let $C \in \mathrm{Cor}(m,n)$. That means there exist unit vectors $\{x_s\}$ and $\{y_t\}$ in $\mathbb{R}^r$, where $r = \mathrm{rank}(C)$, such that $C_{s,t} = \langle x_s, y_t\rangle$ for all s and t. Set $d = 2^{\lceil r/2\rceil}$ and define

$$X_s = \sum_{i=1}^r (x_s)_i \varphi_r(a_i), \quad Y_t = \sum_{i=1}^r (y_t)_i \varphi_r(a_i)^{\mathsf{T}},$$

where φ_r is the representation of $\mathcal{C}(r)$ as defined in (9). With $\psi = \frac{1}{\sqrt{d}}\sum_{i=1}^d e_i \otimes e_i$ one can derive the following identity (see for example [2]):

$$C_{s,t} = \langle x_s, y_t\rangle = \mathrm{Tr}(X_sY_t^{\mathsf{T}})/d = \psi^*(X_s \otimes Y_t)\psi \quad \text{for all} \quad s \in S, t \in T.$$

The eigenvalues of the matrices $\varphi(a_1), \dots, \varphi(a_r)$ lie in $\{-1,1\}$, and the Clifford relations (8) can be used to derive that the eigenvalues of X_s and Y_t also lie in $\{-1,1\}$. Thus, $(\{X_s\}, \{Y_t\}, \psi)$ is a tensor operator representation of C.

(2) $\Rightarrow$ (3) If $(\{X_s\}, \{Y_t\}, \psi)$ is a tensor operator representation of C, then the operators $X_s \otimes I$ and $I \otimes Y_t$ commute, and by using the identity

$$\psi^*(X_s \otimes Y_t)\psi = \mathrm{Tr}((X_s \otimes I)(I \otimes Y_t)\psi\psi^*)$$

we see that $(\{X_s \otimes I\}, \{I \otimes Y_y\}, \psi\psi^*)$ is a pure commuting operator representation.

(3) $\Rightarrow$ (4) This is immediate.

(4) $\Rightarrow$ (1) Suppose $(\{X_s\}, \{Y_t\}, W)$ is a commuting operator representation of C. Since W is positive semidefinite and has trace 1, there exist nonnegative scalars

λ_i and orthonormal unit vectors $\psi_i \in \mathbb{C}^d \otimes \mathbb{C}^d$ such that $W = \sum_i \lambda_i \psi_i \psi_i^*$ and $\sum_i \lambda_i = 1$. Then,

$$C_{s,t} = \mathrm{Tr}(X_s Y_t W) = \sum_i \lambda_i \,\mathrm{Tr}(X_s Y_t \psi_i \psi_i^*) = \sum_i \lambda_i \psi_i^* X_s Y_t \psi_i.$$

So, with

$$x_s = \sum_i \sqrt{\lambda_i} \begin{pmatrix} \mathrm{Re}(X_s \psi_i) \\ \mathrm{Im}(X_s \psi_i) \end{pmatrix} \quad \text{and} \quad y_t = \sum_i \sqrt{\lambda_i} \begin{pmatrix} \mathrm{Re}(Y_t \psi_i) \\ \mathrm{Im}(Y_t \psi_i) \end{pmatrix}$$

we have $C_{s,t} = \langle x_s, y_t \rangle$ and $\|x_s\|, \|y_s\| \leq 1$, and by using the observation in the proof of Lemma 3.2 we can extend the vectors x_s and y_t to unit vectors. □

Remark 4.2. *If C has a tensor operator representation in dimension d, then it has a commuting operator representation by matrices of size d^2.*

The remainder of this section is devoted to showing that there are bipartite correlation matrices for which every operator representation requires a large dimension.

For this we need two more definitions. A commuting operator representation $(\{X_s\}, \{Y_t\}, W)$ is *nondegenerate* if there does not exist a projection matrix $P \neq I$ such that $PWP = W$, $X_s P = P X_s$, and $Y_t P = P Y_t$ for all s and t. It is said to be *Clifford* if there exist matrices $Q \in \mathbb{R}^{m\times m}$ and $R \in \mathbb{R}^{n \times n}$ with all-ones diagonals, such that

$$X_s X_{s'} + X_{s'} X_s = 2Q_{s,s'} I \quad \text{for all} \quad s, s' \in S,$$
$$Y_t Y_{t'} + Y_{t'} Y_t = 2R_{t,t'} I \quad \text{for all} \quad t, t' \in T.$$

We will use the following theorem from Tsirelson as crucial ingredient.

Theorem 4.3 ([21])**.** *If C is an extreme point of $\mathrm{Cor}(m, n)$, then any nondegenerate commuting operator representation of C is Clifford.*

We can now state and prove the main result of this section.

Theorem 4.4. *Let C be an extreme point of $\mathrm{Cor}(m, n)$ and let $r = \mathrm{rank}(C)$. Every commuting operator representation of C uses matrices of size at least $2^{\lfloor r/2 \rfloor}$.*

Proof. Let $(\{X_s\}, \{Y_t\}, W)$ be a commuting operator representation of C where X_s, Y_t and W are matrices of size d, our goal is to show $d \geq 2^{\lfloor r/2 \rfloor}$. If this representation is degenerate, then there exists a projection matrix $P \neq I$ such that $PWP = W$, $X_s P = P X_s$, and $Y_t P = P Y_t$ for all s and t. Let $P = \sum_{i=1}^k v_i v_i^*$ be its spectral decomposition, where the vectors $v_1, \ldots, v_k$ are orthonormal, and set $U = (v_1, \ldots, v_k)$. Then, one can verify that $(\{U^* X_s U\}, \{U^* Y_s U\}, U^* W U)$ is a commuting operator representation of C of smaller dimension. We are proving a lower bound on the dimension, therefore we can assume $(\{X_s\}, \{Y_t\}, W)$ is a nondegenerate commuting operator representation.

By extremality of C we may assume the operator representation is pure. Hence, there is a unit vector ψ such that $W = \psi\psi^*$. This gives

$$C_{s,t} = \mathrm{Tr}(X_s Y_t W) = \psi^* X_s Y_t \psi = \langle x_s, y_t \rangle,$$

where

$$x_s = \begin{pmatrix} \mathrm{Re}(X_s \psi) \\ \mathrm{Im}(X_s \psi) \end{pmatrix} \quad \text{and} \quad y_t = \begin{pmatrix} \mathrm{Re}(Y_t \psi) \\ \mathrm{Im}(Y_t \psi) \end{pmatrix}.$$

These vectors $\{x_s\}$ and $\{y_t\}$ are unit vectors because C is extreme (see the proof of Lemma 3.2), and therefore, they form a C-system.

By Theorem 4.3 the commuting operator representation $(\{X_s\},\{Y_t\},W)$ is Clifford. So, there exist matrices $Q \in \mathbb{R}^{m\times m}$ and $R \in \mathbb{R}^{n\times n}$ with all-one diagonals such that

$$X_sX_{s'} + X_{s'}X_s = 2Q_{s,s'}I \quad \text{for all} \quad s,s' \in S,$$
$$Y_tY_{t'} + Y_{t'}Y_t = 2R_{t,t'}I \quad \text{for all} \quad t,t' \in T.$$

We show that E is an extension of C to the elliptope, where

$$E = \begin{pmatrix} Q & C \\ C^{\mathsf{T}} & R \end{pmatrix}.$$

For this, we have to show $Q_{s,s'} = \langle x_s, x_{s'}\rangle$ and $R_{t,t'} = \langle y_t, y_{t'}\rangle$. Indeed,

$$\begin{aligned}\langle x_s, x_{s'}\rangle + \langle x_{s'}, x_s\rangle &= \mathrm{Re}\,\big(\psi^* X_sX_{s'}\psi + \psi^* X_{s'}X_s\psi\big)\\ &= \mathrm{Re}\,\big(\psi^*(X_sX_{s'} + X_{s'}X_s)\psi\big)\\ &= \mathrm{Re}\,\big(\psi^*(2Q_{s,s'}I)\psi\big) = 2Q_{s,s'},\end{aligned}$$

and in the same way $\langle y_t, y_{t'}\rangle + \langle y_{t'}, y_t\rangle = 2R_{t,t'}$.

By Theorem 3.3 the matrix E is the unique extension of C to the elliptope. Furthermore, Lemma 3.2 tells us that $\mathrm{rank}(Q) = \mathrm{rank}(R) = \mathrm{rank}(C) = r$.

Consider the spectral decomposition of Q: $Q = \sum_{i=1}^r \alpha_i v_i v_i^*$, where the vectors $v_1,\ldots,v_r$ are orthonormal, and consider the algebra $\mathbb{C}\langle A_1,\ldots,A_r\rangle$, where

$$A_i = \frac{1}{\sqrt{\alpha_i}}\sum_{s=1}^m (v_i)_s X_s \quad \text{for} \quad i \in [r].$$

We have

$$\begin{aligned}A_iA_j + A_jA_i &= \frac{1}{\sqrt{\alpha_i\alpha_j}}\sum_{s,s'=1}^m \big((v_i)_s(v_j)_{s'}X_sX_{s'} + (v_j)_s(v_i)_{s'}X_sX_{s'}\big)\\ &= \frac{1}{\sqrt{\alpha_i\alpha_j}}\sum_{s,s'=1}^m (v_i)_s(v_j)_{s'}\,(X_sX_{s'} + X_{s'}X_s)\\ &= \frac{1}{\sqrt{\alpha_i\alpha_j}}\sum_{s,s'=1}^m (v_i)_s(v_j)_{s'}2Q_{s,s'}I = \frac{2}{\sqrt{\alpha_i\alpha_j}}v_i^*Qv_jI = 2\delta_{i,j}I,\end{aligned}$$

which means that $\mathbb{C}\langle A_1,\ldots,A_r\rangle$ is a representation of the Clifford algebra $\mathcal{C}(r)$. Hence, the matrices $A_1,\ldots,A_r$ must have size at least $2^{\lfloor r/2\rfloor}$, which implies that the matrices $\{X_s\}$ and $\{Y_t\}$ have size $d \geq 2^{\lfloor r/2\rfloor}$. ☐

Corollary 4.5. *Let C be an extreme point of $\mathrm{Cor}(m,n)$ and let $r = \mathrm{rank}(C)$. Every tensor operator representation of C has local dimension at least $\sqrt{2}^{\lfloor r/2\rfloor}$.*

Proof. Directly from Theorem 4.4 using Remark 4.2. ☐

5. Matrices with high completely positive semidefinite rank

In this section we prove our main result and construct completely positive semidefinite matrices with exponentially large cpsd-rank. In order to do so we are going to use an addditional link between bipartite correlations and quantum correlations, combined with the fact that quantum correlations arise as projections of completely positive semidefinite matrices. We start with recalling the facts that we need about quantum correlations.

Let A, B, S, and T be finite sets. A function $p\colon A\times B\times S\times T \to [0,1]$ is called a *quantum correlation*, realizable in *local dimension* d, if there exist a unit vector

$\psi \in \mathbb{C}^d \otimes \mathbb{C}^d$ and Hermitian positive semidefinite $d \times d$ matrices X_s^a ($s \in S$, $a \in A$) and Y_t^b ($t \in T$, $b \in B$) satisfying the following two conditions:

$$\sum_{a \in A} X_s^a = \sum_{b \in B} Y_t^b = I \quad \text{for all} \quad s \in S, t \in T, \tag{10}$$

$$p(a,b|s,t) = \psi^*(X_s^a \otimes Y_t^b)\psi \quad \text{for all} \quad a \in A, b \in B, s \in S, t \in T. \tag{11}$$

The next theorem shows a link between quantum correlations and $\mathcal{CS}_+$-matrices. This result can be found in [20, Theorem 3.2] (see also [16]). This link allows us to construct $\mathcal{CS}_+$-matrices with large cpsd-rank by finding quantum correlations that cannot be realized in a small local dimension.

Theorem 5.1. *A function $p\colon A \times B \times S \times T \to [0,1]$ is a quantum correlation that can be realized in local dimension d if and only if there exists a completely positive semidefinite matrix M, with rows and columns indexed by the disjoint union $(A \times S) \sqcup (B \times T)$, satisfying the following conditions:*

$$\text{cpsd-rank}(M) \le d, \tag{12}$$

$$M_{(a,s),(b,t)} = p(a,b|s,t) \quad \textit{for all} \quad a \in A, b \in B, s \in S, t \in T, \tag{13}$$

and

$$\sum_{a \in A, b \in B} M_{(a,s),(b,t)} = \sum_{a,a' \in A} M_{(a,s),(a',s')} = \sum_{b,b' \in B} M_{(b,t),(b',t')} = 1 \tag{14}$$

for all $s, s' \in S$ and $t, t' \in T$.

Next we show how to construct from a bipartite correlation $C \in \mathrm{Cor}(m,n)$ a quantum correlation p, with $|A| = |B| = 2$ and $S = [m]$, $T = [n]$, having the property that the smallest local dimension in which p can be realized is lower bounded by the smallest local dimension of a tensor representation of C.

Lemma 5.2. *Let $C \in \mathrm{Cor}(m,n)$ and assume that each tensor representation of C requires local dimension at least d. There exists a quantum correlation p defined on $\{0,1\} \times \{0,1\} \times [m] \times [n]$, satisfying the relations*

$$C(s,t) = p(0,0|s,t) + p(1,1|s,t) - p(0,1|s,t) - p(1,0|s,t) \ \textit{for}\ s \in [m], t \in [n], \tag{15}$$

that can be realized only in local dimension at least d.

Proof. We first show the existence of a quantum correlation that satisfies (15). Let $C \in \mathrm{Cor}(m,n)$. Theorem 4.1 tells us that there exist an integer d, a unit vector $\psi \in \mathbb{C}^d \otimes \mathbb{C}^d$, and Hermitian $d \times d$ matrices $X_1, \ldots, X_m, Y_1, \ldots, Y_n$, whose spectra are contained in $[-1,1]$, such that $C_{s,t} = \psi^*(X_s \otimes Y_t)\psi$ for all s and t. We define the Hermitian positive semidefinite matrices

$$X_s^a = \frac{I + (-1)^a X_s}{2}, \ Y_t^b = \frac{I + (-1)^b Y_t}{2} \quad \text{for } a, b \in \{0,1\}. \tag{16}$$

Using the fact that $X_s^0 + X_s^1 = Y_t^0 + Y_t^1 = I$, $X_s = X_s^0 - X_s^1$, and $Y_t = Y_t^0 - Y_t^1$, it follows that the function $p(a,b|s,t) = \psi^*(X_s^a \otimes Y_t^b)\psi$ is a quantum correlation that satisfies (15).

Assume that p can be realized in dimension k, we show that $k \ge d$. As p is realizable in dimension k there exist a unit vector $\psi \in \mathbb{C}^k \otimes \mathbb{C}^k$ and Hermitian positive semidefinite $k \times k$ matrices $\{X_s^a\}$ and $\{Y_t^b\}$ such that

$$\sum_{a \in \{0,1\}} X_s^a = \sum_{b \in \{0,1\}} Y_t^b = I \quad \text{for all} \quad s \in S, t \in T,$$

for which we have $p(a,b|s,t) = \psi^*(X_s^a \otimes Y_t^b)\psi$. Observe that the spectrum of the operators X_s^a and Y_t^b is contained in $[0,1]$. We define $X_s = X_s^0 - X_s^1, Y_t = Y_t^0 - Y_t^1$. Then, using (15), we can conclude

$$C_{s,t} = \psi^*(X_s \otimes Y_t)\psi.$$

This means that C has a tensor operator representation in local dimension k and thus, by the assumption of the lemma, $k \geq d$. □

By combining the above with the result of Corollary 4.5 from the previous section we can now prove our main theorem.

Theorem 1.1. *For each positive integer r there exists a completely positive semidefinite matrix M of size $r^2 + r + 2$ with* cpsd-rank$(M) \geq \sqrt{2}^{\lfloor r/2 \rfloor}$.

Proof. Let r be a positive integer and set $n = \binom{r}{2} + 1$ and $d = \sqrt{2}^{\lfloor r/2 \rfloor}$. By Lemma 3.11 there exists an extreme point C of $\mathrm{Cor}(r,n)$ with rank r. Corollary 4.5 tells us that every tensor operator representation of C requires local dimension at least d.

Let $p\colon A \times B \times S \times T \to [0,1]$, with $|A| = |B| = 2$ and $|S| = r$, $|T| = n$, be the quantum correlation constructed from C as indicated in Lemma 5.2. Let M be the completely positive semidefinite matrix constructed from p as indicated in Theorem 5.1, with size $|A||S| + |B||T| = 2(r+n) = r^2 + r + 2$.

Then, by Lemma 5.2, p is not realizable in dimension smaller than d and thus, by Theorem 5.1, cpsd-rank$(M) \geq d$. □

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