Structure of the set of quantum correlators via semidefinite programming

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Quantum information leverages properties of quantum behaviors in order to perform useful tasks such as secure communication and randomness certification. Nevertheless, not much is known about the intricate geometric features of the set quantum behaviors. In this paper we study the structure of the set of quantum correlators using semidefinite programming. Our main results are (i) a generalization of the analytic description by Tsirelson-Landau-Masanes, (ii) necessary and sufficient conditions for extremality and exposedness, and (iii) an operational interpretation of extremality in the case of two dichotomic measurements, in terms of self-testing. We illustrate the usefulness of our theoretical findings with many examples and extensive computational work.

I. INTRODUCTION

Quantum theory distinguishes itself from classically-conceived theories of physics in several ways, most notably in terms of the observable correlations between space-like separated parties. In the seminal work [5], John Bell discovered that quantum theory allows correlations between space-like separated observers beyond those allowed by local realistic classical theories, a property known as “nonlocality”. The existence of nonlocal quantum correlations predicted theoretically by Bell has been confirmed by numerous experiments [14, 19, 35], which have influenced deeply our understanding of the physical world, and have led to real-life applications in cryptography [12] and randomness certification [7] among others.

Despite the usefulness of the nonlocal distributions that can be generated using quantum resources, the structure of the set of quantum distributions is not well understood. Most notably, there are many semidefinite programming hierarchies that approximate the set of quantum correlations from the exterior, but these hierarchies only converge in the limit, e.g., see [10, 28]. In fact, it was shown only recently in [36] that the set of (tensor product) quantum correlations is not closed.

Furthermore, it is known that quantum behaviors are not maximally non-local, and from a foundational perspective, there has been an ongoing research program to identify the physical principles behind quantum theory. Several principles have been proposed, such as information causality [30] and macroscopic locality [29], but none succeeded to single out the set of quantum distributions.

From a practical perspective, to manipulate quantum information, one needs a robust method for identifying quantum systems. This is a challenging task due to the intrinsic probabilistic nature of quantum theory. Motivated by this, there has been extensive work studying the relationship between objects in the theory, namely quantum states and measurements, and the theory’s predictions, namely probabilities of experiments. This direction line of research is known in the literature as quantum tomography whose recent reincarnation is known as self-testing and gate set tomography.

In this work we study the set of quantum correlations by taking a geometric viewpoint. Specifically, as the quantum set is convex, its properties can be understood via various features of its convex geometry, such as its facial structure and its extreme points [12].

The main technical tool used in this work is semidefinite programming, whose relevance is already implicit in the work of Tsirelson [39], a connection that was pursued further in [10, 28]. Specifically, it essentially follows from [39] that the geometry of the set of quantum correlators is the projection of the geometry of the elliptope, a convex set of central interest in combinatorial optimization [9].

The link to semidefinite programming leads to several interesting results. First, we generalize the Tsirelson-Landau-Masanes analytic description for the set of quantum correlators, in the case where at least one party performs at most two dichotomic measurements (Theorem 1). Second, we derive necessary and sufficient conditions for extremality (Theorem 2), and a sufficient condition for exposedness (Theorem 3). Third, we give an operational interpretation of extremality in the case of two dichotomic measurements (Theorem 4).

Our last result is particularly striking as it highlights that natural geometric features of the set of quantum correlators, such as extremality, correspond to important physical and operational properties.

Lastly, we note that the approach of studying the quantum set within the framework of convex analysis was also employed in [15]. Our approach differs in that we use as our main tool properties of semidefinite programming.

We start with a brief review of Bell nonlocality (Section II), followed by the precise definition of the set of quantum correlators—our main object of study—and a characterization via the positive semidefinite matrix completion problem (Section III), which leads to an analytic description (Section IV). Further exploiting this connection, we study the convex geometry of quantum correlators, its extreme points (Section VA) and
exposed points (Section V D), and present a connection between the geometric concept of extremality with the operational task of self-testing (Section V C). Algorithmic results and examples are interspersed in these sections whenever convenient. We conclude the paper with a high level overview of our results and pointers towards future research.

II. BELL NONLOCALITY

Bell experiment. The experimental and mathematical framework for studying behaviors between two space-like separated parties is known as a bipartite Bell experiment. In this setting two parties, called Alice and Bob, perform independently and simultaneously local measurements on their corresponding subsystems and record the resulting outcomes. In this work, we restrict to Bell experiments where the parties can only perform dichotomic (i.e. two-outcome) measurements.

The event that the first party performed measurement $x$ and got outcome $a$, whereas the second party performed measurement $y$ and got outcome $b$ is denoted by $(a, b|x, y)$. The next step is to consider physical theories, that assign probabilities $p(a, b|x, y)$ to all possible events of a Bell experiment. The collection of all joint conditional probabilities $p(a, b|x, y)$ is called a full behavior.

Clearly, for any physical theory, behaviors satisfy non-negativity and normalization conditions, i.e.,

$$ p(a, b|x, y) \geq 0, \forall a, b, x, y, $$

$$ \sum_{a, b} p(a, b|x, y) = 1, \forall x, y. $$

Furthermore, for reasonable physical theory, the behaviors that can be generated between space-like separated parties have the property that each parties local marginal distribution does not depend on the other parties choice of measurement, i.e.,

$$ \sum_{b} p(a, b|x, y) = \sum_{b} p(a, b|x', y'), \forall a, x, y \neq y' \text{ and } $$

$$ \sum_{a} p(a, b|x, y) = \sum_{a} p(a, b|x', y), \forall b, y, x \neq x'. $$

A full behavior that satisfies all the linear constraints given in (1) is called no-signaling. Given a no-signaling behavior, we denote $p_A(a|x)$ and $p_B(b|y)$ the local marginal distributions of Alice and Bob, respectively.

As we only consider dichotomic measurements, we can use an equivalent parametrization of a no-signaling behavior $p(a, b|x, y)$ in terms of average values. Explicitly, for outcome labels $a, b \in \{\pm 1\}$ we use the affine bijection

$$ p(a, b|x, y) \mapsto (c_x, c_y, c_{xy}) $$

where

$$ c_x = \sum_{a \in \{\pm 1\}} a p_A(a|x) \quad c_y = \sum_{b \in \{\pm 1\}} b p_B(b|y), $$

$$ c_{xy} = \sum_{a, b \in \{\pm 1\}} a b p(a, b|x, y). $$

The image of the set of full behaviors under the map (2) is called the set of full correlators, and its elements are denoted by $(c_x, c_y, c_{xy})$. Lastly, the coordinate projection of the set of full correlators on the coordinates $c_{xy}$ is the correlator space and its element are called correlators.

Local behaviors and correlators. A behavior $p(a, b|x, y)$ is called local deterministic if $p(a, b|x, y) = \delta_{a,f(x)}\delta_{b,g(y)}$, where $\delta$ is the Kronecker delta function and $f, g$ are functions from the input set to the output set. Furthermore, a behaviour $p(a, b|x, y)$ is called local, if it can be written as a convex combination of local deterministic behaviours, i.e., $p(a, b|x, y) = \sum \mu_i p_i$, where $\mu \geq 0$, $\sum \mu_i = 1$ and each $p_i$ is local deterministic.

Fixing outcome labels $a, b \in \{\pm 1\}$, the corresponding set of correlators is the convex hull of all $n \times m$ matrices $xy^T$, where $x \in \{\pm 1\}^n \times \{\pm 1\}^m$ and $y \in \{\pm 1\}^m \times \{\pm 1\}^n$. This is known as the cut polytope of the complete bipartite graph $K_{n,m}$ (in $\pm 1$ variables) and is of central importance in the field of combinatorial optimization [9].

Quantum behaviors and correlators. According to the (Hilbert space) axioms of quantum mechanics, a full behavior $p(a, b|x, y)$ is quantum, if there exist a quantum state acting on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, and $\{M_a^x\}$ and $\{M_b^y\}$, local measurements acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, i.e.,

$$ \rho \geq 0 \text{ and } \text{tr}(\rho) = 1; $$

$$ M_a^x \geq 0 \text{ and } \sum_a M_a^x = 1; $$

$$ M_b^y \geq 0 \text{ and } \sum_b M_b^y = 1. $$

such that $p(a, b|x, y) = \text{tr}(M_a^x \otimes M_b^y \rho)$. Equivalently, a full correlator $(c_x, c_y, c_{xy})$ is quantum, if there exist a quantum state $\rho$ acting on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, and $\pm 1$ observables $A_1, ..., A_n, B_1, ..., B_m$ acting on $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively, such that

$$ c_x = \text{tr}(A_x \otimes I_B \rho), \quad x \in [n]; $$

$$ c_y = \text{tr}((I_A \otimes B_y) \rho), \quad y \in [m]; $$

$$ c_{xy} = \text{tr}(\rho A_x \otimes B_y), \quad x \in [n], y \in [m]. $$

The set of quantum correlators, denoted by $\text{Cor}(n, m)$, is the set of all vectors $c_{xy}$ where $c_{xy} = \text{tr}(\rho A_x \otimes B_y)$ for a quantum state $\rho$ and $\pm 1$ observables $A_1, ..., A_n, B_1, ..., B_m$. It is evident that the difference with full correlators lies in the lack of local marginals $a_x, b_y$. Note that the set of quantum correlators is a compact and convex subset of the cube $[-1, 1]^{nm}$. Throughout this work, we arrange the entries of a quantum correlator $c_{xy} \in \text{Cor}(n, m)$ as an $n \times m$ matrix $C$, which we call a quantum correlation matrix. We use the vector and matrix representations interchangeably.
III. LINK TO SEMIDEFINITE PROGRAMMING

A semidefinite program (SDP) is a mathematical optimization problem, where the objective is to optimize a linear function over an affine slice of the cone of positive semidefinite matrices. A SDP in primal canonical form is given by

$$p^* = \sup_X \{ \langle C, X \rangle : X \succeq 0, \langle A_i, X \rangle = b_i \ (i \in [\ell]) \}, \quad (P)$$

where $\langle \cdot, \cdot \rangle$ denotes the trace inner product of matrices, and the generalized inequality $X \succeq 0$ means that the matrix $X$ is positive semidefinite, i.e., it has nonnegative eigenvalues. SDPs are an important generalization of linear programming, which is obtained as a special case when all involved matrices are diagonal. SDPs have significant modeling power, powerful duality theory, and efficient algorithms for solving them.

The link between quantum correlators and SDPs originates in the seminal work of Tsirelson [39, Theorem 2.1]. Specifically, Tsirelson showed that a matrix $C = (c_{xy}) \in [-1,1]^{n \times m}$ is a quantum correlation matrix if and only if there exists a collection of real unit vectors $u_1, \ldots, u_n, v_1, \ldots, v_m$ such that

$$c_{xy} = \langle u_x, v_y \rangle, \text{ for all } x \in [n], y \in [m]. \quad (4)$$

We note that $\langle \cdot, \cdot \rangle$ denotes the canonical inner product of vectors. As a consequence of Tsirelson’s theorem it follows that $C = (c_{xy}) \in [-1,1]^{n \times m}$ is a quantum correlation matrix if and only if the following SDP is feasible:

$$\max_X 0 \quad \text{s.t.} \quad X_{xy} = c_{xy}, \ x \in [n], y \in [m], \quad X_{ii} = 1, \ i \in [n + m], \quad X \in S^{n+m}_+. \quad (5)$$

To establish this equivalence note that if $c_{xy} = \langle u_x, v_y \rangle, \forall x \in [n], y \in [m], \text{ where } \|u_x\| = \|v_y\| = 1$, the Gram matrix $\text{Gram}(u_1, \ldots, u_n, v_1, \ldots, v_m)$ is feasible for $[\delta]$. Conversely, if $X \in S^{n+m}_+$ is feasible for $[\delta]$, by the spectral theorem for real symmetric matrices, there exist unit vectors $u_1, \ldots, u_n, v_1, \ldots, v_m$ such that $X = \text{Gram}(u_1, \ldots, u_n, v_1, \ldots, v_m)$. Clearly, this implies that $c_{xy} = \langle u_x, v_y \rangle, \forall x \in [n], y \in [m]$, and thus $C = (c_{xy})$ is a quantum correlation matrix.

Furthermore, a geometric interpretation of Tsirelson’s theorem is that the set of $n \times m$ quantum correlation matrices $\text{Cor}(n,m)$ is the image of the set of $(n+m) \times (n+m)$ positive semidefinite matrices with diagonal entries equal to one, denoted by $\mathcal{E}_{n+m}$, under the projection

$$\Pi : S^{n+m} \rightarrow \mathbb{R}^{n \times m}, \quad \begin{pmatrix} A & C \\ C^T & B \end{pmatrix} \mapsto C, \quad (6)$$

i.e., we have that $\text{Cor}(n,m) = \Pi(\mathcal{E}_{n+m})$.

Any matrix in $\Pi^{-1}(C) \cap \mathcal{E}_{n+m}$ is called a PSD completion of $C$. Thus, checking whether a matrix $C = (c_{xy}) \in [-1,1]^{n \times m}$ is a quantum correlation matrix reduces to checking that the partially specified matrix $(c_{xy})$ can be completed to a full PSD matrix with diagonal entries equal to one. For example, the CHSH correlator $C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, is quantum, as the corresponding partial matrix

$$\begin{pmatrix} 1 & a & 1/\sqrt{2} & 1/\sqrt{2} \\ a & 1 & 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} & 1 & b \\ 1/\sqrt{2} & -1/\sqrt{2} & b & 1 \end{pmatrix}, \quad (7)$$

admits a PSD completion, obtained for $a = b = 0$.

The problem of completing a partially specified matrix into a full PSD matrix is an important instance of semidefinite programming, referred to as the PSD matrix completion problem, e.g. see [13] and references therein.

One of the most fruitful approaches for studying the PSD matrix completion problem has been the use of graph theory. Specifically, let $G = ([n], E)$ be a simple undirected graph, whose edges encode the positions of the known entries of the matrix. The elliptope or coordinate shadow of a graph $G$, denoted by $\mathcal{E}(G)$, is defined as the image of $\mathcal{E}_n$ under the coordinate projection

$$\Pi_G : S^n \rightarrow \mathbb{R}^E, \quad A \mapsto (A_{ij})_{i,j \in E}. \quad (8)$$

In other words, any vector $a \in \mathcal{E}(G) \subseteq \mathbb{R}^E$ corresponds to a $G$-partial matrix, that admits a completion to a full PSD matrix with diagonal entries equal to one.

The properties and structure of the elliptope of a graph have been studied extensively, e.g. see [9, 11, 17, 38]. By the definition of the elliptope if a graph, it is clear that

$$\text{Cor}(n,m) = \mathcal{E}(K_{n,m}),$$

where $K_{n,m}$ denotes the complete bipartite graph, where the bipartitions have $n$ and $m$ vertices respectively. This link allows us to utilize properties concerning the structure of the elliptope of a graph $\mathcal{E}(G)$, in our study of the structure of the set of quantum correlators.

IV. ANALYTIC DESCRIPTION OF Cor(n,m)

A first property of $\mathcal{E}(G)$ of relevance to this work is that the elliptope of a graph $G = ([n], E)$ is subset of a nonlinear transform of the metric polytope, denoted by $\text{Met}(G)$, which consists of all vectors $x = (x_e) \in \mathbb{R}^E$ satisfying

$$0 \leq x_e \leq 1, \text{ for all } e \in E; \quad (9)$$

$$\sum_{e \in F} x_e - \sum_{e \in C \setminus F} x_e \leq |F| - 1, \quad (10)$$

where $C$ is any cycle in $G$, and $F$ is any odd cardinality subset of $C$. Recall that a cycle in a graph is a sequence of vertices starting and ending at the same vertex, where each two consecutive vertices in the sequence are adjacent.
The relation between $\mathcal{E}(G)$ and $\text{Met}(G)$ is completely understood, e.g. see [22] Theorem 4.7. Specifically, its is known that for any graph $G$, we have the inclusion $\mathcal{E}(G) \subseteq \cos(\pi \text{Met}(G))$. Furthermore, equality holds if and only if the graph $G$ does not have the complete graph on four vertices, denoted by $K_4$, as a minor.

Two observations concerning this result are in order. First, note that the cosine function is applied componentwise, i.e., for a vector $x = (x_e) \in \mathbb{R}^E$ we define $\cos(x) \in \mathbb{R}^E$, where $\cos(x)_e = \cos(x_e)$. Second, a graph $H$ is called a minor of a graph $G$, if $H$ can be obtained from $G$ through a series of edge deletions, edge contractions and isolated node deletions.

Based on this and the fact that $\text{Cor}(n,m) = \mathcal{E}(K_{n,m})$, we now derive an analytic description for $\text{Cor}(n,m)$, whenever $\min\{n,m\} \leq 2$. Indeed, it is easy to check that the complete bipartite graph $K_{n,m}$ has the complete graph on four vertices $K_4$ as minor if and only if $\min\{n,m\} > 2$. Thus, it follows that $\text{Cor}(n,m) = \cos \pi \text{Met}(K_{n,m})$, whenever $\min\{n,m\} \leq 2$. This gives:

**Theorem 1.** For $\min\{n,m\} \leq 2$, we have that $C = (c_{xy}) \in \text{Cor}(n,m)$ if and only if the following linear system is feasible

\[
\begin{align*}
0 & \leq \theta_{xy} \leq \pi, \quad \forall x,y, \\
0 & \leq \theta_{1j} + \theta_{2i} + \theta_{2j} - \theta_{1i} \leq 2\pi, \\
0 & \leq \theta_{1i} + \theta_{2i} + \theta_{2j} - \theta_{1j} \leq 2\pi, \\
0 & \leq \theta_{1i} + \theta_{1j} + \theta_{2j} - \theta_{2i} \leq 2\pi, \\
0 & \leq \theta_{1i} + \theta_{1j} + \theta_{2i} - \theta_{2j} \leq 2\pi,
\end{align*}
\]

where $3 \leq i < j \leq n + 2$ and $\theta_{xy} = \arccos(c_{xy})$.

As an example, in the case of $\text{Cor}(2,2)$, the resulting characterization is known as the Tsirelson-Landau-Masanes criterion, which has been rediscovered numerous times, e.g. see [39, 21 and 25]. To the best of our knowledge, the description for $\text{Cor}(2, n)$ when $n \geq 3$ is new. The proof of Theorem 1 is given in the Appendix.

**V. EXTREMAL AND EXPOSED CORRELATORS**

In this section we use that $\text{Cor}(n,m)$ is a projection of the ellipsope $\mathcal{E}_{n+m}$, to study the convex geometry of $\text{Cor}(n,m)$. We begin with its extreme points (or zero-dimensional faces) and continue with its exposed points.

**A. Extremal correlators**

A matrix $C \in \text{Cor}(n,m)$ is an extreme point of $\text{Cor}(n,m)$ if the equality $C = \lambda C_1 + (1 - \lambda) C_2$, where $\lambda \in (0,1)$ and $C_1, C_2 \in \text{Cor}(n,m)$, implies $C = C_1 = C_2$.

The set of extreme points of $\text{Cor}(n,m)$, denoted by $\text{ext}(\text{Cor}(n,m))$, is important for the following reasons. Firstly, since the set of quantum correlators is compact (i.e. closed & bounded) and convex, by the Krein-Milman Theorem (e.g. see [4] Theorem 3.3], $\text{Cor}(n,m)$ is equal to the convex hull of its extreme points.

Secondly, Tsirelson showed that any quantum realization of an extremal correlator in $\text{Cor}(n,m)$ corresponds to a complex representation of an appropriate Clifford algebra [39 Theorem 3.1]. As a consequence, depending on the parity of the rank of an extremal correlator $C$, it either has one or two “non-equivalent” (up to arbitrary unitaries) quantum representations. In modern language, Tsirelson’s work specialized to the case of even-rank extremal correlators is a self-testing statement, a connection we pursue further Section V C.

In this section we derive an exact characterization for extremality in $\text{Cor}(n,m)$, in terms of the PSD matrix completion problem. This fact essentially follows from the work of Tsirelson [39, 40], and was also recently noted in [10 Theorem 3.3]. The main tool in the proof is a set of necessary conditions for extremality derived by Tsirelson, which we have collected in Theorem 8 in the Appendix.

**Theorem 2.** A correlator $C \in \text{Cor}(n,m)$ is extremal if and only if $C$ has a unique PSD completion $\hat{C} \in \mathcal{E}_{n+m}$, and furthermore,

\[
\text{rank}(\hat{C} \circ \hat{C}) = \left(\frac{\text{rank}(\hat{C}) + 1}{2}\right),
\]

where $\circ$ denotes the componentwise product of matrices.

**Proof.** The forward implication is a consequence of Theorem 8 (iii), combined with the following characterization of extreme points of the ellipsope $\mathcal{E}_n$:

\[
E \in \text{ext}(\mathcal{E}_n) \iff \text{rank}(E \circ E) = \left(\frac{\text{rank}(E) + 1}{2}\right).
\]

For the converse direction, by assumption we have that $\Pi^{-1}(C) \cap \mathcal{E}_{n+m} = \{\hat{C}\}$, where the map $\Pi$ was defined in (6). Furthermore, the rank assumption on $\hat{C}$ combined with (13) imply that $\hat{C} \in \text{ext}(\mathcal{E}_{n+m})$. Since $C \in \text{ext}(\text{Cor}(n,m))$ if and only if $\Pi^{-1}(C)$ is a face of $\mathcal{E}_{n+m}$, e.g. see [27 Lemma 2.4], we conclude that $C \in \text{ext}(\text{Cor}(n,m))$ (as an extreme point is a face). \qed

Illustrating the usefulness of Theorem 2 we now show the extremality of various quantum correlator matrices.

The only other technique available in the literature for showing extremality of a quantum correlator is via the notion of self-testing. Specifically, it was shown in [16 Proposition C.1] that a full correlator $(c_x, c_y, c_{xy})$ which is a self-test, is also necessarily an extreme point of the set of full correlators. It is easy to verify that this argument remains valid for correlators, i.e., if $C \in \text{Cor}(n,m)$ is a self-test, it is also an extreme point of $\text{Cor}(n,m)$.

**Example 1:** The CHSH correlator $C = \frac{1}{\sqrt{2}} \left( \begin{smallmatrix} 1 & -1 \\ 1 & 1 \end{smallmatrix} \right)$, is well-known to be a self-test (e.g. see [34 Theorem 4.1]),
and thus, it is an extreme point of Cor(2, 2). To recover this by Theorem 2, we first show that the partial matrix

\[
\begin{pmatrix}
1 & a & 1/\sqrt{2} & 1/\sqrt{2} \\
a & 1 & 1/\sqrt{2} & -1/\sqrt{2} \\
1/\sqrt{2} & 1/\sqrt{2} & 1 & b \\
1/\sqrt{2} & -1/\sqrt{2} & b & 1
\end{pmatrix}
\]

(14)

admits a unique PSD completion. Indeed, consider an arbitrary completion and let \(x_1, x_2, y_1, y_2\) be the vectors in a Gram decomposition. Define \(z_+ = \frac{x_1 + x_3}{\sqrt{2}}\) and \(z_- = \frac{x_1 - x_3}{\sqrt{2}}\). Clearly, \(\langle z_+, z_- \rangle = 0\). Furthermore, \(\langle y_1, z_+ \rangle = 1\) and \(\langle y_1, z_- \rangle = 0\). Since \(\|y_1\| = 1\) it follows that \(y_1 = \frac{z_+}{\|z_+\|}\), and in the same manner we get that \(y_2 = \frac{z_-}{\|z_-\|}\). This implies that \(b = \langle y_1, y_2 \rangle = 0\). Similarly, we get that \(a = 0\). Thus the unique PSD completion is

\[
\hat{C} = \begin{pmatrix}
1 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\
0 & 1 & 1/\sqrt{2} & -1/\sqrt{2} \\
1/\sqrt{2} & 1/\sqrt{2} & 1 & 0 \\
1/\sqrt{2} & -1/\sqrt{2} & 0 & 1
\end{pmatrix}.
\]

(15)

Lastly, as \(\text{rank}(\hat{C}) = 2\) and \(\text{rank}(\hat{C} \circ \hat{C}) = 3\), it follows by Theorem 2 that \(C \in \text{ext}(\text{Cor}(2, 2))\).

**Example 2:** The Mayers-Yao correlator [26]

\[
C = \begin{pmatrix}
1 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\
0 & 1 & 1/\sqrt{2} & 1/\sqrt{2} \\
1/\sqrt{2} & 1/\sqrt{2} & 1 & 0 \\
1/\sqrt{2} & 1/\sqrt{2} & 0 & 1
\end{pmatrix},
\]

(16)

is a self-test (e.g. see [34, Theorem 4.2]), and thus, it is an extreme point of Cor(3, 3). To recover this by Theorem 2, we first check that the corresponding partial matrix

\[
\begin{pmatrix}
1 & a & b & 1 & 0 & 1/\sqrt{2} \\
a & 1 & c & 0 & 1 & 1/\sqrt{2} \\
b & c & 1 & 1/\sqrt{2} & 1/\sqrt{2} & 1 \\
a & 0 & 1/\sqrt{2} & 1 & d & e \\
1/\sqrt{2} & 1/\sqrt{2} & d & e & f & 1 \\
1/\sqrt{2} & 1/\sqrt{2} & e & f & 1 & 1
\end{pmatrix}.
\]

(17)

admits a unique PSD completion. To see this, consider an arbitrary PSD completion and let \(x_1, x_2, x_3, y_1, y_2, y_3\) be a Gram decomposition. Since \(\|x_1\| = \|y_1\| = 1\) and \(\langle x_1, y_1 \rangle = 1\), we have that \(x_1 = y_1\). Similarly, we get that \(x_2 = y_2\). These two conditions imply that

\begin{align*}
a &= \langle x_1, x_2 \rangle = \langle x_1, y_2 \rangle = 0, \\
b &= \langle x_1, x_3 \rangle = \langle y_1, x_3 \rangle = 1/\sqrt{2}, \\
c &= \langle x_2, x_3 \rangle = \langle y_2, x_3 \rangle = 1/\sqrt{2}, \\
d &= \langle y_1, y_2 \rangle = \langle x_1, x_2 \rangle = 0, \\
e &= \langle y_1, y_3 \rangle = \langle x_1, x_3 \rangle = 1/\sqrt{2}, \\
f &= \langle y_2, y_3 \rangle = \langle x_2, y_3 \rangle = 1/\sqrt{2}.
\end{align*}

(18)

Summarizing, the unique PSD completion of \(C\) is

\[
\hat{C} = \begin{pmatrix}
1 & 0 & 1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} \\
0 & 1 & 1/\sqrt{2} & 1/\sqrt{2} & 0 & 1/\sqrt{2} \\
1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} & 1 & 0 \\
1/\sqrt{2} & 1/\sqrt{2} & 0 & 1/\sqrt{2} & 1 & 0 \\
1/\sqrt{2} & 1/\sqrt{2} & 0 & 1/\sqrt{2} & 1/\sqrt{2} & 1
\end{pmatrix}.
\]

(19)

Lastly, since \(\text{rank}(\hat{C}) = 2\) and \(\text{rank}(\hat{C} \circ \hat{C}) = 3\), it follows by Theorem 2 that \(C \in \text{ext}(\text{Cor}(2, 3))\).

**Example 3:** The quantum correlator

\[
C = \frac{1}{2} \begin{pmatrix}
1 & 1 & 1 \\
1 & 1 & -2
\end{pmatrix}.
\]

is a self-test [11], and thus, an extreme point of Cor(2, 2). It can be easily checked that the corresponding partial matrix has a unique PSD completion given by

\[
\hat{C} = \begin{pmatrix}
1 & -1/2 & 1/2 & 1/2 \\
-1/2 & 1/2 & -1 & 1/2 \\
1/2 & 1/2 & -1 & 1 \\
1/2 & -1/2 & 1 & 1
\end{pmatrix}.
\]

As \(\text{rank}(\hat{C}) = 2\) and \(\text{rank}(\hat{C} \circ \hat{C}) = 3\), it follows that \(C \in \text{ext}(\text{Cor}(2, 2))\).

**Extreme points of Cor(2, 2).** In this section we give an explicit characterization of the extreme points of Cor(2, 2), in terms of the angle parametrization from Theorem 1.

**Theorem 3.** Let \(C = (c_{xy}) \in \text{Cor}(2, 2)\) and define \(\theta_{xy} = \arccos(c_{xy})\) for all \(x \in \{1, 2\}, y \in \{3, 4\}\).

(i) If \(\text{rank}(C) = 1\), then \(C\) is extreme iff it is local deterministic, i.e., \(C = xy^T\), for \(x, y \in \{\pm 1\}^2\).

(ii) If \(\text{rank}(C) = 2\), then \(C\) is extreme iff it saturates exactly one of the inequalities

\[
0 \leq \sum_{xy \neq x'y'} \theta_{xy} - \theta_{x'y'} \leq 2\pi,
\]

and at most one of the inequalities

\[
0 \leq \theta_{xy} \leq \pi,
\]

where \(x, x' \in \{1, 2\}, y, y' \in \{3, 4\}\).

The case rank(\(C\)) = 1 is straightforward so we mainly focus on the case rank(\(C\)) = 2. To prove extremality, we use the assumptions of the theorem to prove the existence of a unique completion that satisfies (12). Extremality then follows by Theorem 2.

For the converse direction, we translate the assumption of extremality, namely unique completability and the rank condition (12) to the level of the parameters \(\theta_{xy} = \arccos(c_{xy})\). As it turns out, these assumptions imply that the unspecified parameters \(\theta_{12}, \theta_{34}\) are uniquely determined in any completion. In turn, this shows that one cycle inequality and at most one box inequality are tight. The details are given in the Appendix.

**B. Verifying extremality computationally**

The examples given in the previous section illustrate the usefulness of the characterization of extremality given in Theorem 2. Nevertheless, it is not clear whether Theorem 2 leads to an algorithm for testing extremality, as
a priori, it is not immediately obvious how to systematically check whether the corresponding completion problem has a unique solution. We address this issue using the rich duality theory enjoyed by SDPs, summarized in Theorems 3 and 7 in the Appendix.

Back to the completion problem, given \( C = (c_{xy}) \in \text{Cor}(n,m) \), its PSD completions coincide with the set of solutions of the SDP feasibility problem \( \text{(5)} \).

Next, we dualize the SDP \( \text{(5)} \). For this, we first write \( \text{(5)} \) in primal canonical form (recall \( \text{(A2)} \)), i.e.,

\[
\begin{align*}
\max_X & \quad 0 \\
\text{s.t.} & \quad \langle E_{xy}, X \rangle = c_{xy}, \ x \in [n], \ y \in [m], \\
& \quad \langle E_{ii}, X \rangle = 1, \ i \in [n+m], \\
& \quad X \in S_+^{n+m}, \\
\end{align*}
\]

where \( E_{xy} = \frac{1}{2}(e_x e_y^T + e_y e_x^T) \).

The dual of the SDP \( \text{(20)} \) is given by

\[
\begin{align*}
\inf_{\lambda,Z} & \quad \sum_{i=1}^{n+m} \lambda_i + \sum_{x=1}^{n} \sum_{y=1}^{m} \lambda_{xy} c_{xy} \\
\text{s.t.} & \quad \sum_{i=1}^{n+m} \lambda_i E_{ii} + \sum_{x=1}^{n} \sum_{y=1}^{m} \lambda_{xy} E_{xy} = Z \in S_+^{n+m}. \\
\end{align*}
\]

Note that the SDP \( \text{(21)} \) admits a positive definite feasible solution, e.g. obtained by setting \( \lambda_{xy} = 0, \forall x, y \) and taking \( \lambda_i \) to be sufficiently large. Furthermore, by weak duality for SDPs (cf. Theorem 3 (i)), we have that \( 0 = p^* \leq d^*, \) i.e., \( d^* > -\infty \). By strong duality for SDPs (cf. Theorem 3 (ii)), these two properties imply that the value of the dual SDP \( \text{(21)} \) is equal to zero, i.e. \( d^* = 0 \). Furthermore, \( d^* = 0 \) is clearly attained, e.g. take \( \lambda_i = \lambda_{xy} = 0 \). Lastly, as \( C \in \text{Cor}(n,m) \) by assumption, the primal SDP \( \text{(5)} \) is also attained. Thus, to show that the SDP \( \text{(5)} \) has a unique solution, it suffices to exhibit a nondegenerate optimal solution for \( \text{(21)} \).

Specializing the definition of dual nondegeneracy for SDPs (recall \( \text{(A2)} \)) to a dual feasible solution \( (\lambda,Z) \) for the SDP \( \text{(21)} \), this is equivalent to asking that \( M = 0 \) is the only solution of the system:

\[
\begin{align*}
MZ &= 0; \\
M_{ii} &= 0, \ 1 \leq i \leq m+n; \\
M_{ij} &= 0, \ 1 \leq i \leq n, \ n \leq j \leq n+m. \\
\end{align*}
\]

An important observation is that \( \text{(22)} \) is a linear program in the entries of the symmetric matrix variable \( M \in S_+^{n+m} \), and thus, it is efficiently solvable.

We are now ready to describe an algorithmic procedure for determining extremality of a given \( C \in \text{Cor}(n,m) \), based on Theorem 2 and the notion of SDP nondegeneracy. For the convenience of the reader, the algorithm is summarized in a flow chart in Fig. 1.

**Step 1:** We solve the pair of primal-dual SDPs \( \text{(20)} \) and \( \text{(21)} \), to get \( X_{\text{opt}} \) and \( Z_{\text{opt}} \), respectively.

**Step 2:** We check whether \( Z_{\text{opt}} \) is dual non-degenerate, i.e., we check whether \( M = 0 \) is the only solution to the linear programming problem \( \text{(22)} \) (where \( Z = Z_{\text{opt}} \)).

**Step 3a:** If \( Z_{\text{opt}} \) is non-degenerate, then \( X_{\text{opt}} \) is the unique solution of the primal SDP \( \text{(20)} \) by Theorem 7. Lastly, we check whether \( \text{rank}(X_{\text{opt}} \circ X_{\text{opt}}) = (\text{rank}(X_{\text{opt}})) + 1) \); if this holds then \( C \) is extreme, and if it fails, \( C \) is not extreme.

**Step 3b:** If \( Z_{\text{opt}} \) is degenerate and

\[
\text{rank}(X_{\text{opt}}) + \text{rank}(Z_{\text{opt}}) = m + n, \tag{23}
\]

we conclude that \( C \) is *not extreme*. Indeed, if \( C \) was extreme, by Theorem 2, \( X_{\text{opt}} \) would be the unique solution of the SDP \( \text{(20)} \). As \( X_{\text{opt}}, Z_{\text{opt}} \) satisfy \( \text{(23)} \), by Theorem 7 (ii) the matrix \( Z_{\text{opt}} \) would be dual nondegenerate optimal solution, a contradiction.

**Step 3c:** If \( Z_{\text{opt}} \) is degenerate and

\[
\text{rank}(X_{\text{opt}}) + \text{rank}(Z_{\text{opt}}) < m + n, \tag{24}
\]

our procedure is inconclusive.

Note that by weak duality for SDPs, we always have that \( \text{rank}(X_{\text{opt}}) + \text{rank}(Z_{\text{opt}}) \leq m + n \). Thus, condition \( \text{(23)} \) fails if and only if condition \( \text{(24)} \) holds.

We implemented this procedure on MATLAB using the YALMIP package and Mosek as the solver 1. Furthermore, we tested the performance of the procedure on randomly generated extremal points of \( \text{Cor}(2,2) \). Specifically, with randExtremeCorr22.m, we generate a random point in \( \text{ExtCor}(2,2) \) by randomly picking three angles, \( \theta_1, \theta_2, \theta_3 \in (0, \pi) \), and setting \( \phi = \theta_1 + \theta_2 + \theta_3 \). If \( \phi < \pi \) or \( 2\pi < \phi < 3\pi \), we set the fourth angle \( \theta_4 = \phi \), otherwise, we discard this instance. Then, by Theorem 3 the correlator corresponding to \( \cos(\theta_1, \theta_2, \theta_3, \theta_4) \) is extremal in \( \text{Cor}(2,2) \). We applied our procedure, called extremeCorr.m, on 1000 extremal points generated by randExtremeCorr22.m. In all instances, our algorithm correctly detected that the generated points are indeed extreme.

**C. Operational interpretation of extremality**

It turns out that the geometric concept of extremality has a nice operational interpretation. We now explain the connection with the task of self-testing, which has been hinted several times in the previous sections.

Self-testing, also referred to as device-independent characterization of the state and the measurements, or simply blind tomography, captures the idea that certain correlations between space-like separated parties predicted by quantum theory determine the state and the measurement up to local isometries and other irrelevant degrees of freedom.

The term self-testing was introduced in the work by Mayers and Yao [26]. Nevertheless, the idea underlying self-testing was rediscovered earlier numerous times in the literature, for example in the works of Tsirelson [39].
Summers-Werner [37], and Popescu-Rohrlich [31]. The interested reader is referred to [34] for a general survey, and [6] [20] for more recent developments.

To formally define self-testing, recall that a quantum realization of $C_t$ is a quantum realization of $C$ if, for any $A_x \otimes B_y$ there exist isometries $V_A : \mathcal{H}_A \otimes \mathcal{H}_A^r \to \mathcal{H}_A$ and $V_B : \mathcal{H}_B \otimes \mathcal{H}_B^r \to \mathcal{H}_B$ and a unit vector $\psi'' \in \mathcal{H}_A^r \otimes \mathcal{H}_B^r$ such that

$$
\psi'' = (V_A \otimes V_B)(\psi \otimes \psi'').
$$

Furthermore, we say that $C$ is a self-test if it self-tests some quantum realization $(\mathcal{H}_A, \mathcal{H}_B, \psi, \{A_x\}_{x}, \{B_y\}_{y})$.

In the following theorem we give a geometric characterization of self-testing for the special case of $\text{Cor}(2,2)$.

**Theorem 4.** Let $C \in \text{Cor}(2,2)$ with rank$(C) = 2$. The following are equivalent:

1. $C$ is an extreme point of $\text{Cor}(2,2)$.
2. $C$ self-tests the singlet.
3. $C$ is a self-test.

**Proof.** In [11] Theorem 1] it is shown that a rank two correlator $C \in \text{Cor}(2,2)$ self-tests the singlet if and only if, $C$ saturates exactly one of the inequalities

$$
-\pi \leq \sum_{x \neq x'} \arcsin(c_{xy}) - \arcsin(c_{xy}) \leq \pi, \forall x', y',
$$

and at most one of the inequalities

$$
-\pi/2 \leq \arcsin(c_{xy}) \leq \pi/2, \forall x, y,
$$

where $x, x' \in \{1, 2\}$, $y, y' \in \{3, 4\}$. Using that $\arccos(x) + \arcsin(x) = \frac{\pi}{2}$ and $\theta_{xy} = \arccos(c_{xy})$, the equivalence between (ii) and (ii) follows from Theorem 3(ii). Lastly, the equivalence between (ii) and (iii) is a special case of [39] Theorem 3.2.}

**D. Exposed correlators**

An exposed face of $\text{Cor}(n,m)$ is a subset $F \subseteq \text{Cor}(n,m)$ for which there exists a matrix $A \in \mathbb{R}^{n \times m}$ such that $F = \text{argmax}\{\langle A, X \rangle : X \in \text{Cor}(n,m)\}$. A matrix $C \in \text{Cor}(n,m)$ is an exposed point of $\text{Cor}(n,m)$ if the singleton $\{C\}$ is an exposed face of $\text{Cor}(n,m)$, i.e., there exists $A \in \mathbb{R}^{n \times m}$ such that

$$
\{C\} = \text{argmax}\{\langle A, X \rangle : X \in \text{Cor}(n,m)\}.
$$
Setting $b = \max \{ \langle A, X \rangle : X \in \text{Cor}(n, m) \}$, $C$ is an exposed point of $\text{Cor}(n, m)$ if the following two properties hold: (i) $\langle A, X \rangle \leq b$, for all $X \in \text{Cor}(n, m)$ and (ii) $\langle A, X \rangle = b$ if and only if $X = C$. In this setting, we say that the hyperplane $H = \{ X \in \mathbb{R}^{n \times m} : \langle A, X \rangle = b \}$ exposes the point $C$.

The exposed points of a convex set are always extreme, but the converse is not always true. An example of such a point is the Hardy behavior \([13]\), which is extreme point of the set of full behaviors (as it is a self-test \([33]\), but was recently shown to be non exposed \([15]\).

In this section, we use again SDP duality theory to give a sufficient condition for a point $C \in \text{Cor}(n, m)$ to be exposed. Our main tool is the following result.

**Theorem 5.** Let $C^* = (c_{xy}^*)$ be an extreme point of $\text{Cor}(n, m)$ and $Z^* = \sum_{i=1}^{n+m} \lambda_i^* E_{ii} + \sum_{x=1}^{n} \sum_{y=1}^{m} \lambda_{xy}^* E_{xy}$ a dual optimal solution for (21).

(i) The hyperplane

$$H = \left\{ (c_{xy}) : -\sum_{x=1}^{n} \sum_{y=1}^{m} \lambda_{xy}^* c_{xy} = \sum_{i=1}^{n+m} \lambda_i^* \right\},$$

supports the set Cor$(n, m)$ at the point $C^*$, i.e.,

$$-\sum_{x=1}^{n} \sum_{y=1}^{m} \lambda_{xy}^* c_{xy} \leq \sum_{i=1}^{n+m} \lambda_i^*, \forall C \in \text{Cor}(n, m), \text{ and}$$

$$-\sum_{x=1}^{n} \sum_{y=1}^{m} \lambda_{xy}^* c_{xy} = \sum_{i=1}^{n+m} \lambda_i^*.$$

(ii) Furthermore, if the homogeneous linear system

$$MZ^* = 0, \quad M_{ii} = 0, \quad 1 \leq i \leq n + m,$$ \hspace{1cm} (30)

in the symmetric matrix variable $M \in S^{n+m}$ has only the trivial solution $M = 0$, then, the hyperplane $H$ given in (29) exposes the point $C^*$.

**Proof.** Recall that the solution set of (20) coincides with the set of PSD completions of $C^*$. As $C^*$ is extreme, by Theorem 2, it has a unique PSD completion $\hat{C}^* \in S^{n+m}_+$, i.e., $\hat{C}^*$ is the unique solution of the SDP (20).

We have already seen that the values of (20) and (21) coincide, and both are attained. Consequently, as $C^*$ and $Z^*$ are primal-dual optimal, we have $\langle C^*, Z^* \rangle = 0$ (cf. Theorem 5 (iii)). Expanding this we get

$$\sum_{i=1}^{n+m} \lambda_i^* + \sum_{x=1}^{n} \sum_{y=1}^{m} \lambda_{xy}^* c_{xy} = 0.$$

Lastly, consider an arbitrary $C \in \text{Cor}(n, m)$ and let $\hat{C}$ be one of its PSD completions. As the PSD cone is self-dual we get that $\langle \hat{C}, Z^* \rangle \geq 0$, and expanding, this gives

$$\sum_{i=1}^{n+m} \lambda_i^* + \sum_{x=1}^{n} \sum_{y=1}^{m} \lambda_{xy}^* c_{xy} \geq 0.$$
Using these two vectors we define

\[ Z^* = v_1 v_1^\top + v_2 v_2^\top = \begin{pmatrix} 1 & 0 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & 1 & 0 \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 1 & 0 \end{pmatrix}. \]

Next, we show that \( Z^* \) is dual optimal for (21). Indeed, by construction \( Z^* \) is feasible for (21), and satisfies \( \langle \mathcal{C}, Z^* \rangle = \langle \mathcal{C}, v_1 v_1^\top \rangle + \langle \mathcal{C}, v_2 v_2^\top \rangle = 0 \). As \( C \) is optimal for (5), Theorem 6 (iii) implies that \( Z^* \) is dual optimal.

Having established that \( Z^* \) is dual optimal, Theorem 4 implies that the hyperplane \( c_{11} + c_{12} + c_{21} - c_{22} \leq 2\sqrt{2} \) supports \( \text{Cor}(2, 2) \) at the CHSH correlator. Lastly, to prove that this hyperplane exposes the CHSH correlator, by Theorem 5 (ii), it suffices to show that the homogeneous linear system (30) only admits the trivial solution. A straightforward calculation reveals this is the case.

**Example 5.** We show that the hyperplane

\[ -12\sqrt{2}c_{14} + 4c_{15} - 4\sqrt{2}c_{16} + 4c_{24} - 12\sqrt{2}c_{25} - 4\sqrt{2}c_{26} - 4\sqrt{2}c_{34} - 4\sqrt{2}c_{35} + 2(2 - 3\sqrt{2})c_{36} \leq 6(5\sqrt{2} + 2), \]

exposes the Mayers-Yao correlator (10). In Example 2, we showed that the SDP (20) has the unique solution

\[ X^* = \begin{pmatrix} 1 & 0 & \frac{1}{\sqrt{2}} & 1 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & \frac{1}{\sqrt{2}} & 0 & 1 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 1 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 1 \\ 1 & 0 & \frac{1}{\sqrt{2}} & 1 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & \frac{1}{\sqrt{2}} & 0 & 1 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 1 & \frac{1}{\sqrt{2}} & 1 & 1 \end{pmatrix}. \] (35)

Note that \( \text{rank}(X^*) = 2 \), and in fact, its column space is spanned by the first two columns. Thus, its nullspace has dimension four, and a basis is given by the vectors:

\[ v_1 = (-1, -1, -1, 1, 1, 1)^\top, \]
\[ v_2 = (-1, 1, 0, 1, -1, 0)^\top, \]
\[ v_3 = (1, 1, -\sqrt{2}, 1, 1, -\sqrt{2})^\top, \]
\[ v_4 = (1, 1, -1, -1, 1, 1)^\top. \]

Using these vectors we define,

\[ Z^* = 2\sqrt{2}v_1 v_1^\top + (3\sqrt{2} + 1)v_2 v_2^\top + v_3 v_3^\top + \sqrt{2}v_4 v_4^\top \]
\[ = \begin{pmatrix} 2(3\sqrt{2}+1) & 0 & 0 & -6\sqrt{2} & 2 & -2\sqrt{2} \\ 0 & 2(3\sqrt{2}+1) & 0 & 2 & -6\sqrt{2} & -2\sqrt{2} \\ 0 & 0 & 3\sqrt{2}+2 & -2\sqrt{2} & -2\sqrt{2} & 2-3\sqrt{2} \\ 0 & 0 & 0 & 3\sqrt{2}+2 & -2\sqrt{2} & -2\sqrt{2} \\ 0 & 0 & 0 & 0 & 3\sqrt{2}+2 & -2\sqrt{2} \\ 0 & 0 & 0 & 0 & 0 & 3\sqrt{2}+2 \end{pmatrix}. \]

By construction, \( Z^* \) is positive semidefinite, feasible for (21), and satisfies \( \langle X^*, Z^* \rangle = 0 \). Consequently, by Theorem 6 (iii) we get that \( Z^* \) is dual optimal for (21) and thus, by Theorem 5 (i), we see that (34) is a valid hyperplane for \( \text{Cor}(3, 3) \). It remains to show that the hyperplane (34) exposes the Mayers-Yao correlator. For this, by Theorem 5 (ii), suffices to show that the linear system (30) only admits the trivial solution. An easy calculation shows that this is indeed the case.

**Verifying exposedness computationally.** Theorem 5 leads to an algorithm for checking whether a given extremal correlator \( C \) is exposed. This is summarized below:

**Step 1.** Solve the SDP (21) to find an optimal solution \( Z^* = \sum_{i=1}^{n+m} \lambda_i^* E_{ii} + \sum_{i=1}^{m} \lambda_i^* E_{xy} \). 

**Step 2.** Solve the SDP (33) to find an optimal solution \( Z \). If \( Z \) is non-degenerate then \( C \) is exposed. If \( Z \) is degenerate, the test is inconclusive.

We implemented this procedure on 1000 randomly generated extremal correlators from \( \text{Cor}(2, 2) \). In all instances, our algorithm concluded that the corresponding correlators were also exposed. The algorithm for generating the random instances is implemented in randExtremeCorr.m and the entire procedure is implemented in exposedCorr.m. Our computations suggest that for \( \text{Cor}(2, 2) \), most extreme points are also exposed [1].

**VI. CONCLUSIONS AND FUTURE WORK**

In this paper we studied geometric features of the set of quantum correlators using semidefinite programming. Our starting point is that the set of quantum correlations can be seen as the projection of the feasible region of a semidefinite program, known as the ellipsoid. This connection leads to a characterization of its boundary, which generalizes the well-known Tsirelson-Landau-Masanes criterion (Theorem 1). Furthermore, based on this connection, we were able to translate results concerning the geometry of ellipsoids to the set of quantum correlations. The first question we considered was to characterize its extreme points, or equivalently its zero-dimensional faces. We managed to give a complete characterization by making a link to the positive semidefinite matrix completion problem (Theorem 2). Furthermore, for the simplest Bell scenario we determined an explicit characterization of its extreme points (Theorem 3). Next, we gave a sufficient condition for a correlator to be the exposed (Theorem 5). Our numerical experiments suggest that most nonlocal extreme points of \( \text{Cor}(2, 2) \) are in fact exposed. Lastly, we show that in the simplest Bell scenario, the geometric property of extremality coincides with the operational task of self-testing (Theorem 4).

Our investigations in this paper naturally lead to several future directions:

- Can one obtain further analytic characterizations for scenarios not captured by Theorem 1? Can one generalize to multipartite correlation scenarios?
- What is the facial structure of the set of quantum correlations?
- In the set of full quantum behaviors, is extremality still equivalent to self-testing? If not, is extremality equivalent to self-testing with global isometries?
The first two questions are evident; let us comment on the third one. Here self-testing with global isometries is a similar notion to self-testing, but with the “gauge” equivalence being relaxed to arbitrary global isometries (yet still preserve the observed behavior). In other words, the (equivalence) orbit of each realization is larger as we allow global isometries in addition to local isometries. Note that self-testing with global isometries implies the usual self-testing, but the converse does not hold in general. Now it turns out that Theorem 4 can be strengthened by adding the equivalence:

(iv) $C$ is a self-testing with global isometries.

Thus, extremality gives a stronger property than (usual) self-testing in this context. We leave the study of these concepts and their relationships as future work.

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Appendix A: Semidefinite programming

In this section we briefly collect all the tools from SDP duality theory that we use in this paper. For proofs of these facts and additional details, the interested reader is referred to [8].

Theorem 6. Consider a pair of primal-dual SDPs

\[ p^* = \sup_X \{ \langle C, X \rangle : X \succeq 0, (A_i, X) = b_i (i \in [\ell]) \}, \quad (P) \]
\[ d^* = \inf_{y, Z} \left\{ \sum_{i=1}^{\ell} b_i y_i : \sum_{i=1}^{\ell} y_i A_i - C = Z \succeq 0 \right\}. \quad (D) \]

The following properties hold:

(i) (Weak duality) Let $X, (y, Z)$ be a pair of primal-dual feasible solutions for $(P)$ and $(D)$ respectively. Then, $\langle C, X \rangle \leq \sum_{i=1}^{\ell} b_i y_i$, i.e., $p^* \leq d^*$.

(ii) (Optimality condition) Let $X, (y, Z)$ be a pair of primal-dual feasible solutions for $(P)$ and $(D)$ respectively. If $\langle C, X \rangle = \sum_{i=1}^{\ell} b_i y_i$, then we have that $p^* = d^*$ and furthermore, $X$ and $(y, Z)$ are primal-dual optimal solutions respectively.

(iii) (Complementary slackness) Let $X, (y, Z)$ be a pair of primal-dual feasible solutions for $(P)$ and $(D)$ respectively. Under the assumption that $p^* = d^*$ we have that $X, (y, Z)$ are primal-dual optimal if and only if $(X, Z) = 0$.

(iv) (Strong duality) Assume that $d^* > -\infty$ (resp. $p^* < +\infty$) and that $(D)$ (resp. $(P)$) is strictly feasible. Then $p^* = d^*$ and furthermore, the primal (resp. dual) optimal value is attained.

Given a pair of primal-dual SDPs $(P)$ and $(D)$, a primal feasible solution $X$ is called primal nondegenerate if

\[ T_X + \text{span}\{A_1, \ldots, A_\ell\} = \mathcal{S}^n, \quad (A1) \]

and a dual feasible solution $(y, Z)$ is dual nondegenerate if

\[ T_Z + \text{span}\{A_1, \ldots, A_\ell\} = \mathcal{S}^n, \quad (A2) \]

where $T_X$ is the tangent space on the manifold of symmetric $n \times n$ matrices with rank equal to rank$(Z)$, at the point $Z$, and the sum of two vectors spaces denotes the linear span of their union.

A concrete expression for the tangent space is

\[ T_Z^* = \{ M \in \mathcal{S}^n : MZ = 0 \}, \]

e.g., see [2] or [21 Lemma 7.1.1].

The next result summarizes sufficient conditions for the unicity of optimal solutions to SDPs identified in [2], which we use extensively throughout this work.

Theorem 7. Consider a pair of primal-dual SDPs $(P)$ and $(D)$, where we assume that their optimal values are equal and that both are attained. We have that:

(i) If $(P)$ has a nondegenerate optimal solution, $(D)$ has a unique optimal solution. Symmetrically, if $(D)$ has a nondegenerate optimal solution, then $(P)$ has a unique optimal solution.

(ii) Furthermore, let $X, (y, Z)$ be a pair of primal-dual optimal solutions that satisfy

\[ \text{rank}(X) + \text{rank}(Z) = n, \]

a property known as strict complementarity. Then, if $X$ is the unique optimal solution for $(P)$, $(y, Z)$ is dual nondegenerate. Symmetrically, if $(y, Z)$ is the unique optimal for $(D)$, $X$ is primal nondegenerate.

Appendix B: Necessary conditions for extremality in the set of quantum correlators

In this section we collect several useful properties of extreme points of Cor$(n, m)$, identified in the seminal work of Tsirelson [30, 31]. For a more modern proof of these facts the reader is referred to [32].

A family of vectors $u_1, \ldots, u_n, v_1, \ldots, v_m$ is called a C-system of $C \subset \text{Cor}(n, m)$ if they satisfy $\|u_i\| \leq 1$, $\|v_j\| \leq 1$, and $c_{xy} = \langle u_x, v_y \rangle$, $\forall x \in [n], y \in [m]$. 

Theorem 8. For any $C \in \text{ext}(\text{Cor}(n,m))$ we have:

(i) All $C$-systems are necessarily unit vectors;

(ii) For any $C$-system $\{u_1, \ldots, u_n, v_1, \ldots, v_m\}$ we have that $\text{span}\{u_i\}_{i=1}^n = \text{span}\{v_j\}_{j=1}^m$;

(iii) $C$ admits a unique PSD completion, i.e., there exists a unique matrix $\hat{C} \in \mathcal{E}_{n+m}$ with $\hat{C} = (C, C^- B) \in \mathcal{E}_{n+m}$. Furthermore, we have that $\hat{C} \in \text{ext}(\mathcal{E}_{n+m})$ and $\text{rank}(\hat{C}) = \text{rank}(A) = \text{rank}(B) = \text{rank}(C)$.

We note that the proof of Theorem 8 establishes the following chain of implications (i) $\Rightarrow$ (ii) $\Rightarrow$ (iii). To the best of our knowledge, it is not known whether any of these three conditions is equivalent to extremality.

Appendix C: Properties of PSD completions

In this section we collect certain properties of PSD completions, which we use in the proof of Theorem 8. Recall that any vector $x = (x_c) \in \mathcal{E}(G)$ corresponds to a partial $G$-matrix that admits a PSD completion to a full PSD matrix with diagonal entries equal to one.

As any principal submatrix of a PSD matrix is also PSD, a necessary condition for $a \in \mathcal{E}(G)$ is that the restriction of $a$ to any completely specified principal submatrix is PSD. In other words, if $K$ is a clique in $G$, i.e., a fully connected subgraph of $G$, the restriction of $x$ to $K$, denoted by $x_K$, should lie in $\mathcal{E}(K)$.

This necessary condition turns out to be sufficient if and only if the graph $G$ is chordal, i.e., every circuit of length at least four in $G$ has a chord.

Theorem 9. [17] Graph $G$ is chordal if and only if $\mathcal{E}(G) = \{x \in \mathbb{R}^E : x_K \in \mathcal{E}(K) \text{ for each clique } K \subseteq G\}$.

We also need the following result, which gives an explicit description of $\mathcal{E}(K_3)$.

Theorem 10. [3] Let $0 \leq \theta_1, \theta_2, \theta_3 \leq \pi$. Then, the matrix

$$C = \begin{pmatrix} 1 & \cos \theta_1 & \cos \theta_3 \\ \cos \theta_1 & 1 & \cos \theta_2 \\ \cos \theta_3 & \cos \theta_2 & 1 \end{pmatrix}$$

is positive semidefinite if and only if

$$\begin{align*}
\theta_1 &\leq \theta_2 + \theta_3, & \theta_2 &\leq \theta_1 + \theta_3, & (C1) \\
\theta_3 &\leq \theta_1 + \theta_2, & \theta_1 + \theta_2 + \theta_3 &\leq 2\pi. & (C2)
\end{align*}$$

Furthermore, $C$ is singular if and only if one of the above inequalities holds with equality.

Based on the previous two results, we now prove the following:

Lemma 11. Let $C \in [-1,1]^{2 \times 2}$ and set $\theta_{xy} = \cos^{-1}(c_{xy}) \in [0, \pi]$, for $x \in \{1,2\}$, $y \in \{3,4\}$. Then, $C$ has a PSD completion if and only if:

$$\max\{\theta_{31} - \theta_{41}, |\theta_{32} - \theta_{42}|\} \leq \min\{\theta_{31} + \theta_{41}, \theta_{32} + \theta_{42}, 2\pi - (\theta_{31} + \theta_{41}), 2\pi - (\theta_{32} + \theta_{42})\}. \quad (C3)$$

Furthermore, assuming that (C3) holds, for any PSD completion of $C$, we have that $\theta_{34} = \arccos(c_{34})$ lies in the interval (C3). Conversely, for any $\theta$ in the interval (C3), there exists a PSD completion of $C$ with $\theta_{34} = \theta$.

Proof. Let $K_{2,2}$ be the graph with vertex set $\{1,2,3,4\}$ and edges $\{(1,3), (1,4), (2,3), (2,4)\}$. By definition of the ellipse of a graph, $C \in \mathcal{E}(K_{2,2})$ if and only if there exists $c_{34} \in [0, \pi]$ such that $\{(C, c_{34}) \in \mathcal{E}(K_{2,2} \cup \{3,4\})\}$. Nevertheless, the graph $K_{2,2} \cup \{3,4\}$ is chordal, and thus, by Theorem 9 we have that $C \in \mathcal{E}(K_{2,2})$ if and only if there exists $c_{34} \in [-1,1]$ such that $\{(c_{13}, c_{14}, c_{34}) \in \mathcal{E}(K_3) \text{ and } (c_{23}, c_{24}, c_{34}) \in \mathcal{E}(K_3)\}$. Lastly, by Theorem 10 these two conditions are equivalent to the existence of $\theta_{34} \in [0, \pi]$ satisfying the following sixteen inequalities:

$$\begin{align*}
\theta_{13} &\leq \theta_{14} + \theta_{34}, & \theta_{23} &\leq \theta_{24} + \theta_{34} \\
\theta_{14} &\leq \theta_{13} + \theta_{34}, & \theta_{24} &\leq \theta_{23} + \theta_{34} \\
\theta_{34} &\leq \theta_{13} + \theta_{14}, & \theta_{34} &\leq \theta_{23} + \theta_{24} \\
\theta_{13} + \theta_{14} + \theta_{34} &\leq 2\pi, & \theta_{23} + \theta_{24} + \theta_{34} &\leq 2\pi.
\end{align*} \quad (C4)$$

Eliminating $\theta_{34}$ from the system (C4) we get (C3). □

Appendix D: Proof of Theorem 1

Let $K_{2,n}$ be the complete bipartite graph, where the first bipartition has two vertices labelled $\{1,2\}$ and the second bipartition has $n$ vertices labelled $\{3, \ldots, n+2\}$. As $K_{2,n}$ has no $K_4$ minor, by [22] Theorem 4.7 we have that $\text{Cor}(2,n) = \cos \pi(\text{Met}(K_{2,n}))$. Setting $\theta_{xy} = \arccos(c_{xy})$, we get that $c = (c_{xy}) \in \text{Cor}(2,n)$ if and only if there exists $a = (a_{xy}) \in \text{Met}(K_{2,n})$ such that $c_{xy} = \cos(\pi a_{xy})$, i.e.,

$$\frac{\theta_{xy}}{\pi} \in \text{Met}(K_{2,n}).$$

The box constraints for $\text{Met}(K_{2,2})$ give

$$0 \leq \theta_{xy} \leq \pi, \forall x,y.$$  

We continue with the cycle inequalities for $\text{Met}(K_{2,n})$. Note that for each $3 \leq i < j \leq n+2$, the graph $K_{2,n}$ contains one cycle of length four, namely $C = (1,i,j,2)$. The cycle inequality for $F = \{1i\}$ gives

$$\theta_{1i} - \theta_{1j} - \theta_{2i} - \theta_{2j} \leq 0,$$

and the cycle inequality for $C \setminus F$ gives

$$\theta_{1j} + \theta_{2i} + \theta_{2j} - \theta_{1i} \leq 2\pi.$$
Summarizing, \( c = (c_{xy}) \in \text{Cor}(2,n) \) if and only if
\[
0 \leq \theta_{xy} \leq \pi, \quad \forall x, y, \\
0 \leq \theta_{ij} + \theta_{st} + \theta_{xj} - \theta_{ii} \leq 2\pi, \\
0 \leq \theta_{ti} + \theta_{st} + \theta_{xj} - \theta_{ij} \leq 2\pi, \\
0 \leq \theta_{ii} + \theta_{ij} + \theta_{st} - \theta_{st} \leq 2\pi,
\]
where \( 3 \leq i < j \leq n + 2 \).

**Appendix E: Proof of Theorem 3**

**Part (i).** Let \( C \in \text{Cor}(n, m) \) with \( \text{rank}(C) = 1 \). We show that \( C \) is an extreme point if and only if \( C = xy^\top \), for some \( x \in \{\pm 1\}^n \), \( y \in \{\pm 1\}^m \).

First, assume that \( C = xy^\top \), where \( x \in \{\pm 1\}^n \), \( y \in \{\pm 1\}^m \), and consider a convex combination
\[
C = \sum_k \lambda_k C^k, \quad \text{where} \quad \sum_k \lambda_k = 1, \quad \lambda_k \geq 0, \tag{E1}
\]
where the matrices \( C^k \) lie in \( \text{Cor}(n, m) \), i.e., \( C^k_{ij} = \langle u_i^k, v_j^k \rangle \), where \( \| u_i^k \| = \| v_j^k \| = 1 \). Note that
\[
1 = C_{ij} = |x_iy_j| = \left| \sum_k \lambda_k C^k_{ij} \right| = \left| \sum_k \lambda_k \langle u_i^k, v_j^k \rangle \right| \tag{E2}
\leq \sum_k \lambda_k \| \langle u_i^k, v_j^k \rangle \| \leq \sum_k \lambda_k = 1, \tag{E3}
\]
and thus we have equality throughout. In particular, we get that \( \sum_k \lambda_k \| \langle u_i^k, v_j^k \rangle \| = 1 \), and as \( \| \langle u_i^k, v_j^k \rangle \| \leq 1 \), this implies that \( \| \langle u_i^k, v_j^k \rangle \| = 1 \), for all \( k, i, j \). In other words, all matrices \( C^k \) have entries \( \pm 1 \). Lastly, by \( \text{E1} \) we get that \( C^k = xy^\top \) for all \( k \), and thus \( C \) is extremal.

Conversely, let \( C \) is a rank-one extreme point of \( \text{Cor}(n, m) \). In this setting, we have already mentioned that \( C \) admits a unique PSD completion \( \tilde{C} \in \mathcal{E}_{n+m} \) with \( \tilde{C} = (C, B) \in \mathcal{E}_{n+m} \), and furthermore, \( \tilde{C} \in \text{ext}(\mathcal{E}_{n+m}) \) and \( \text{rank}(\tilde{C}) = \text{rank}(A) = \text{rank}(B) = \text{rank}(C) \), e.g., see [32] Lemma 2.5. By the assumptions we have that \( \text{rank}(C) = 1 \), and thus \( \text{rank}(\tilde{C}) = 1 \), i.e.,
\[
\tilde{C} = \begin{pmatrix} x \\ y \end{pmatrix} \begin{pmatrix} x^\top \\ y \end{pmatrix} \in \mathcal{E}_{n+m}.
\]
Since \( \tilde{C} \in \mathcal{E}_{n+m} \), it follows that \( x_i^2 = y_i^2 = 1 \). In turn, this shows that \( C = xy^\top \) where \( x \in \{\pm 1\}^n \), \( y \in \{\pm 1\}^m \).

**Part (ii).** Let \( C = (c_{12}, c_{14}) \in \text{Cor}(2, 2) \) with \( \text{rank}(C) = 2 \), and set \( \theta_{xy} = \arccos(c_{xy}) \in [0, \pi] \) for all \( x, y \). We show that \( C \) is an extreme Cor(2, 2) if and only if it satisfies exactly one of the cycle inequalities
\[
0 \leq \sum_{xy \neq x'y'} \theta_{xy} - \theta_{x'y'} \leq 2\pi, \quad x, x' \in \{1, 2\}, \quad y, y' \in \{3, 4\},
\]
and at most one of the box inequalities
\[
0 \leq \theta_{xy} \leq \pi, \quad x = 1, 2, \quad y = 3, 4.
\]

First, assuming that \( C \) saturates exactly one cycle inequality and at most one box inequality, we show that \( C \) is extremal. To show extremality, by Theorem 2 it suffices to show that \( C \) has a unique PSD completion \( \tilde{C} \), that furthermore satisfies \( \text{rank}(\tilde{C}) = 1 \). For this, given an arbitrary PSD completion of the matrix \( C \):
\[
\begin{pmatrix} 1 & c_{12} & c_{13} & c_{14} \\ c_{12} & 1 & c_{23} & c_{24} \\ c_{13} & c_{23} & 1 & c_{34} \\ c_{14} & c_{24} & c_{34} & 1 \end{pmatrix},
\]
we show that \( c_{12} \) and \( c_{34} \) are uniquely determined. For concreteness, assume that the tight cycle inequality is:
\[
\theta_{13} + \theta_{23} + \theta_{24} - \theta_{14} = 0. \tag{E5}
\]
This assumption is without loss of generality, as all cycle inequalities are equivalent up to permuting the parties and relabelling the outcomes. In the optimization community this is known as the “switching symmetry” of the cut polytope [4].

The fact that this equality leads to a unique completion should be evident by Lemma 11. However, let us be even more explicit and show that the unknown entries \( c_{12}, c_{34} \) are completely determined by this equation. Summing the two triangle inequalities
\[
-\theta_{13} - \theta_{23} + \theta_{12} \leq 0 \quad \text{and} \quad -\theta_{24} - \theta_{12} + \theta_{14} \leq 0, \tag{E6}
\]
we get that
\[
\theta_{13} + \theta_{23} + \theta_{24} - \theta_{14} \geq 0, \tag{E7}
\]
which combined with \( \text{E5} \) implies that
\[
\theta_{12} = \theta_{13} + \theta_{23} = \theta_{14} - \theta_{24}. \tag{E8}
\]
Indeed, if either of the triangle inequalities in \( \text{E6} \) were strict, then \( \text{E7} \) would also be a strict inequality, contradicting \( \text{E5} \). Similarly, using the two triangle inequalities
\[
-\theta_{23} - \theta_{24} + \theta_{34} \leq 0 \quad \text{and} \quad -\theta_{34} - \theta_{13} + \theta_{14} \leq 0 \tag{E9}
\]
we get that
\[
\theta_{34} = \theta_{23} + \theta_{24} = \theta_{14} - \theta_{13}. \tag{E10}
\]
Taking cosines in \( \text{E8} \) and \( \text{E10} \), we see that the two unspecified entries \( c_{12} \) and \( c_{34} \) in \( \text{E4} \) are uniquely determined. Specifically, we have:
\[
c_{12} = \cos(\theta_{12}) = c_{13}c_{23} - \sqrt{(1 - c_{13}^2)(1 - c_{23}^2)}; \tag{E11}
\]
\[
c_{34} = \cos(\theta_{34}) = c_{23}c_{24} - \sqrt{(1 - c_{23}^2)(1 - c_{24}^2)}; \tag{E12}
\]
where we used that $\theta_{13}, \theta_{14}, \theta_{23}, \theta_{24} \in [0, \pi]$. Summarizing, $C$ has a PSD unique completion, denoted by $\hat{C}$.

The last step of the proof is to show that $\text{rank}(\hat{C} \circ \hat{C}) = 2^{\text{rank}(\hat{C})+1}$. For this, let $x_1, \ldots, x_4$ be a Gram decomposition of $\hat{C}$. By (E5), these four vectors span either a 1-dimensional or a 2-dimensional linear space. In particular, by projecting onto their linear span we may assume that they in fact lie in $\mathbb{R}^2$. Thus, for the rank of $C$ there are two cases to consider: $\text{rank}(\hat{C}) \in \{1, 2\}$.

If $\text{rank}(\hat{C}) = 1$, since $\text{rank}(C) \leq \text{rank}(\hat{C})$ we have that $\text{rank}(C) = 1$, contradicting the assumption that $\text{rank}(C) = 2$. Thus we have that $\text{rank}(\hat{C}) = \text{rank}(C) = 2$. By Theorem 2, it remains to show that

$$\text{rank}(\hat{C} \circ \hat{C}) = \text{dim span}(x_1 x_1^\top, x_2 x_2^\top, x_3 x_3^\top, x_4 x_4^\top) = 3.$$  

Note that $x_1$ is not parallel to $x_2$, for otherwise, the second row of $C$ would be a multiple of the first one, contradicting the assumption $\text{rank}(C) = 2$. Similarly, $x_3$ is not parallel to $x_4$. Thus, the sets $\{x_1, x_2\}$ and $\{x_3, x_4\}$ are basis for $\mathbb{R}^2$. Furthermore, a simple calculation shows that

$$x_3 = \frac{\sin(\theta_{13}) x_1 + \sin(\theta_{23}) x_2}{\sin(\theta_{13} + \theta_{23})}, \quad (E13)$$

and

$$x_4 = \frac{\sin(\theta_{14}) x_1 + \sin(\theta_{24}) x_2}{\sin(\theta_{14} + \theta_{24})}. \quad (E14)$$

For example, to see (E13), expand $x_3$ in the $\{x_1, x_2\}$ basis, i.e., $x_3 = \lambda x_1 + \mu x_2$. Taking inner products with $x_1$ and $x_2$, and eliminating $\mu$ in the resulting linear system, we get that $\lambda = (\cos(\theta_{13}) - \cos(\theta_{23}) \cos(\theta_{12}))/\sin^2(\theta_{12})$. Lastly, substituting $\theta_{12} = \theta_{13} + \theta_{23}$, it follows that $\lambda = \sin(\theta_{13})/\sin(\theta_{13} + \theta_{23})$. Combining (E13) and (E14) we get:

$$x_3 x_3^\top = \frac{\sin^2(\theta_{13}) x_1 x_1^\top + \sin^2(\theta_{23}) x_2 x_2^\top + 2 \sin(\theta_{13}) \sin(\theta_{23}) (x_1 x_2^\top + x_2 x_1^\top)}{\sin(\theta_{13} + \theta_{23})}, \quad (E15)$$

$$x_4 x_4^\top = \frac{\sin^2(\theta_{14}) x_1 x_1^\top + \sin^2(\theta_{24}) x_2 x_2^\top + 2 \sin(\theta_{14}) \sin(\theta_{24}) (x_1 x_2^\top + x_2 x_1^\top)}{\sin(\theta_{14} + \theta_{24})}. \quad (E16)$$

Next we show that

$$x_1 x_2^\top + x_2 x_1^\top \notin \text{span}(x_1 x_1^\top, x_2 x_2^\top). \quad (E17)$$

Wlog we may assume that $x_1 = (1, 0)^\top$. This is because, for any unitary operator $U$, the vectors $U x_1, U x_2, U x_3, U x_4$ also define a Gram decomposition of $\hat{C}$. Furthermore, as $x_1 = (1, 0)^\top$, we have that $x_2 = (\cos(\theta_{12}), \sin(\theta_{12}))^\top$, and consequently,

$$x_1 x_2^\top + x_2 x_1^\top = \begin{pmatrix} 2 \cos(\theta_{12}) & \sin(\theta_{12}) \\ \sin(\theta_{12}) & 0 \end{pmatrix}, \quad (E18)$$

$$x_1 x_1^\top = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (E19)$$

$$x_2 x_2^\top = \begin{pmatrix} \cos^2(\theta_{12}) & \cos(\theta_{12}) \sin(\theta_{12}) \\ \cos(\theta_{12}) \sin(\theta_{12}) & \sin^2(\theta_{12}) \end{pmatrix}. \quad (E20)$$

As $\sin^2(\theta_{12}) = 0$ (since $x_1 \parallel x_2$) we see that (E17) holds.

Lastly, note that either $\sin(\theta_{13}) \sin(\theta_{23}) = 0$ or $\sin(\theta_{14}) \sin(\theta_{24}) = 0$. Indeed, if both are zero, we would have two tight box constraints, contradicting the hypothesis. Wlog say that $\sin(\theta_{13}) \sin(\theta_{23}) \neq 0$. Since $x_1 x_2^\top + x_2 x_1^\top \notin \text{span}(x_1 x_1^\top, x_2 x_2^\top)$, it follows by (E15) that $x_3 x_3^\top \notin \text{span}(x_1 x_1^\top, x_2 x_2^\top)$, and thus dim span$(x_1 x_1^\top, x_2 x_2^\top, x_3 x_3^\top, x_4 x_4^\top) \geq 3$. On the other hand, by (E15) and (E16) it follows that dim span$(x_1 x_1^\top, x_2 x_2^\top, x_3 x_3^\top, x_4 x_4^\top) \leq 3$.

We now prove the converse direction of the theorem. Say that $C$ is a rank two extreme point of Cor$(2, 2)$. By Lemma 32, Lemma 2.5], $C$ has a unique PSD completion $\hat{C}$, where rank$(\hat{C}) = \text{rank}(C) = 2$ and rank$(\hat{C} \circ \hat{C}) = 3$.

First, note that under the assumptions of the theorem there can be at most one tight box constraint. Indeed, having two (or more) tight box constraints implies that $x_1, x_2, x_3, x_4$ consist of two pairs of parallel vectors, which contradicts the fact that span$(x_1 x_1^\top, x_2 x_2^\top, x_3 x_3^\top, x_4 x_4^\top) = 3$. In turn, the fact that we have at most one tight box constraint implies that at most one cycle inequality can be tight. For concreteness, say that $\theta_{14} = \theta_{13} + \theta_{23} + \theta_{24}$ and $\theta_{13} = \theta_{14} + \theta_{23} + \theta_{24} - 2\pi$. Substituting the second equation into the first one we get that $\theta_{23} + \theta_{24} = \pi$, which when substituted back into the first equation gives that $\theta_{14} = \theta_{13} + \pi$. In turn, using that $\theta_{13}, \theta_{14} \in [0, \pi]$, this implies that $\theta_{14} = \pi, \theta_{13} = 0$, i.e., we have two tight box constraints, a contradiction. Thus, it remains to exhibit one tight cycle inequality.

By assumption $C$ is extreme, and thus, it admits a unique PSD completion, i.e., there exists a unique choice for $c_{12}$ and $c_{34}$ that makes the partial matrix (E4) PSD. In particular, there exists a unique choice for the value of $\theta_{34} = \arccos(c_{34})$. We are now ready to conclude the proof of our theorem.

We have already noted that under the assumptions of the theorem, there exists a unique choice for the value of $\theta_{34} = \arccos(c_{34})$. Consequently, by Lemma 11, the interval specified in (C3) should reduce to a single point, i.e., the two endpoints should coincide. This happens iff one expression from the lower bound in (C3) is equal to another expression from the upper bound in (C3).
We consider two cases. First, if these two inequalities have disjoint support, we get a tight cycle inequality. For example, from the equality \( \theta_{31} + \theta_{32} = \theta_{42} \) we get the tight cycle inequality \( \theta_{31} = \theta_{32} + \theta_{42} \). Second, if the two inequalities have the same support, we get a tight box inequality. In turn, this gives a tight cycle inequality. For example, the equality \( \theta_{31} = \theta_{32} + \theta_{42} \) gives the tight box inequality \( \theta_{32} = \pi \). As rank(\( C \)) = 2, all size three minors of \( C \) are singular. In particular, the minor \( C[2, 3, 4] \) is singular, and thus, by Theorem 10, one of the triangle inequalities for \( (2, 3, 4) \) is tight. Using that \( \theta_{32} = \pi \), combined with the fact that we can have at most one box inequality, we get that \( \theta_{34} + \theta_{24} = \pi \). Lastly, the minor \( C[1, 3, 4] \) is also singular, and again by Theorem 10 one of the triangle inequalities for \( (1, 3, 4) \) is tight. For example, if \( \theta_{13} + \theta_{14} = \theta_{34} \), by eliminating \( \theta_{34} \) we get that \( \theta_{13} + \theta_{14} = \pi - \theta_{24} \), which is the tight cycle inequality \( \theta_{13} + \theta_{14} + \theta_{24} = \theta_{32} \).

Let us conclude with a remark that Part (ii) can be proved with a purely algebraic argument, i.e., never use the Gram vectors, by using the fact that rank of a matrix \( M \) is the largest order of any non-zero minor in \( M \). The advantage of this algebraic argument is to eliminate any kind of doubt caused by appeal to geometric intuitions.

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