EXTREME POINTS OF MATRIX CONVEX SETS, FREE SPECTRAHEDRA AND DILATION THEORY

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ABSTRACT. For matrix convex sets a unified geometric interpretation of notions of extreme points and of Arveson boundary points is given. These notions include, in increasing order of strength, the core notions of "Euclidean" extreme points, "matrix" extreme points, and "absolute" extreme points. A seemingly different notion, the "Arveson boundary", has by contrast a dilation theoretic flavor. An Arveson boundary point is an analog of a (not necessarily irreducible) boundary representation for an operator system. This article provides and explores dilation theoretic formulations for the above notions of extreme points.

The scalar solution set of a linear matrix inequality (LMI) is known as a spectrahedron. The matricial solution set of an LMI is a free spectrahedron. Spectrahedra (resp. free spectrahedra) lie between general convex sets (resp. matrix convex sets) and convex polyhedra (resp. free polyhedra). As applications of our theorems on extreme points, it is shown the polar dual of a matrix convex set K is generated, as a matrix convex set, by finitely many Arveson boundary points if and only if K is a free spectrahedron; and if the polar dual of a free spectrahedron K is again a free spectrahedron, then at the scalar level K is a polyhedron.

1. INTRODUCTION

Spectrahedra, the solution sets of linear matrix inequalities (LMIs), play a central role in semidefinite programming, convex optimization and in real algebraic geometry [BPR13, Nem06]. They also figure prominently in the study of determinantal representations [Brä11, NT12, Vin93], the solution of the Lax conjecture [HV07] and in the solution of the Kadison-Singer paving conjecture [MSS15]. The use of LMIs is a major advance in systems engineering in the past two decades [BGFB94, SIG97]. Free spectrahedra, obtained by substituting matrix tuples instead of scalar tuples into an LMI, arise canonically in the theory of operator algebras, systems and spaces and the theory of matrix convex sets. Indeed, free spectrahedra

are the prototypical examples of matrix convex sets over $\mathbb{R}^g$. They also appear in systems engineering, particularly in problems governed by a signal flow diagram (see [dOHMP09]).

Extreme points are an important topic in convexity; they lie on the boundary of a convex set and capture many of its properties [Bar02]. For a spectrahedron Ramana-Goldman [RG95] gave a basic characterization of its Euclidean or classical extreme points. For matrix convex sets, operator algebras, systems, and operator spaces, it is natural to consider *quantized* analogs of the notion of an extreme point. In [WW99] the notion of a matrix extreme point of a compact matrix convex set K was introduced and their result that the matrix extreme points span in the sense that their closed matrix convex hull is K (see also [Far04]) is now a foundation of the theory of matrix convex sets. However, a proper subset of matrix extreme points might also have the spanning property. One smaller class (introduced by Kleski [Kls14]), we call absolute extreme points, is closely related to a highly classical object, the Arveson boundary.

For operator algebras, systems and spaces *in infinite dimensions* Arveson's notion [Arv69] of an (irreducible) boundary representation (introduced as a noncommutative analog of peak points of function algebras) is entirely satisfactory [Ham79, DM05, Arv08, DK15, FHL+] in that they span the set of which they are the boundary. For matrix convex sets generally and free spectrahedra in particular, where the action takes place at matrix levels and does not pass to operators, the situation is less clear. In the finite-dimensional context it is not known whether there are sufficiently many Arveson boundary points (or absolute extreme points) of a set to span the set. Indeed, the issue of whether there is a natural notion of quantized extreme points for matrix convex sets that is minimal (w.r.t. spanning) remains unresolved (see for instance the discussion in [Far04]). Fritz, Netzer and Thom [FNT+] use extreme points to investigate when an abstract operator system has a finite-dimensional concrete realization.

In this article, in the context of matrix convex sets over $\mathbb{R}^g$, we provide geometric unified interpretations of Arveson boundary points, absolute extreme points, matrix extreme points and Euclidean extreme points, giving them all dilation-theoretic interpretations (see Theorem 1.1). This theory of extreme points occupies the majority of the paper.

Next we give some applications of this theory. We establish, in Theorem 1.2 an analog of a result of Kleski [Kls14, Corollary 2.4]: a matrix convex set K over $\mathbb{R}^g$ is spanned by finitely many of its Arveson boundary points if and only if the polar dual K° is a free spectrahedron. As a consequence, in Corollary 6.3 we show if the polar dual of a free spectrahedron K is again a free spectrahedron, then at the scalar level K is a polyhedron. Further we show the spin disk [HKMS+, DDSS+] in two variables provides a non-trivial example of a free spectrahedron that is spanned by its Arveson boundary. In another direction, we show using the Arveson boundary that a natural construction of a matrix convex hull fails.

In the remainder of this introduction, we state, with some precision, our main results along the way introducing the necessary notations and definitions.

1.1. **Notation.** Given positive integers g and n, let $\mathbb{S}_n^g$ denote the set of g-tuples $X = (X_1, \ldots, X_g)$ of complex $n \times n$ self-adjoint matrices and let $\mathbb{S}^g$ denote the sequence $(\mathbb{S}_n^g)_n$. A subset $\Gamma \subseteq \mathbb{S}^g$ is a sequence $\Gamma = (\Gamma(n))_n$ such that $\Gamma(n) \subseteq \mathbb{S}_n^g$ for each n. The set Γ **closed with respect to direct sums** if for each pair of positive integers m and n and each $X \in \Gamma(n)$ and $Y \in \Gamma(m)$,

$$(1.1) \qquad X \oplus Y := \left(\begin{pmatrix} X_1 & 0 \\ 0 & Y_1 \end{pmatrix}, \ldots, \begin{pmatrix} X_g & 0 \\ 0 & Y_g \end{pmatrix} \right) \in \Gamma(n + m).$$

Likewise Γ is **closed with respect to unitary similarity** if

$$U^* X U := (U^* X_1 U, \ldots, U^* X_g U) \in \Gamma(n)$$

for each positive integer n, each $n \times n$ unitary matrix U and each $X \in \Gamma(n)$. A subset $\Gamma \subseteq \mathbb{S}^g$ is a **graded set** if it is closed with respect to direct sums and it is a **free set** if it is also closed with respect to unitary similarity. Often naturally occurring free sets are also closed with respect to restrictions to reducing subspaces. A free set Γ is **fully free** if it is **closed with respect to reducing subspaces**: if $X \in \Gamma(n)$ and $\mathscr{H} \subseteq \mathbb{C}^n$ is reducing for X of dimension m and the isometry $V : \mathbb{C}^m \to \mathbb{C}^n$ has range $\mathscr{H}$, then $V^* X V \in \Gamma(m)$. Free semialgebraic sets (see [HKM16, HM12] for instance), namely the positivity sets of free matrix-valued symmetric polynomials are fully free. The set $\Gamma \subseteq \mathbb{S}^g$ is **bounded** if there is a $C \in \mathbb{R}_{>0}$ such that $C - \sum X_j^2 \succeq 0$ for all $X \in \Gamma$. We call Γ **closed** (resp. **open**, **compact**) if each $\Gamma(n) \subseteq \mathbb{S}_n^g$ is closed (resp. open, compact). We refer the reader to [Voi10, KVV14, MS11, Pop10, AM15, BB07, BKP16] for a systematic study of free sets and free function theory.

1.2. **Matrix convex sets and extreme points.** A tuple $X \in \mathbb{S}_n^g$ is a **matrix convex combination** of tuples $Y^1, \ldots, Y^N$ with $Y^\ell \in \mathbb{S}_{n_\ell}^g$ if there exist $V_\ell : \mathbb{C}^n \to \mathbb{C}^{n_\ell}$ with

$$(1.2) \qquad X = \sum_{j=1}^N V_\ell^* Y^\ell V_\ell \qquad \text{and} \qquad \sum_{j=1}^N V_\ell^* V_\ell = I_n.$$

The matrix convex combination (1.2) is **proper** provided each V_ℓ is surjective. In this case, $n \geq n_\ell$ for each ℓ. We will say that a convex combination of the form (1.2) is **weakly proper** if all of the V_j are nonzero.

A graded set K is **matrix convex** if it is closed under matrix convex combinations. Equivalently, K is matrix convex if it is graded and for each pair of positive integers $m \leq n$, each $X \in K(n)$ and each isometry $V : \mathbb{C}^m \to \mathbb{C}^n$, the tuple $V^* X V \in K(m)$; i.e., K is closed with respect to **isometric conjugation**. In particular, a matrix convex set is a free set.

Suppose K is a free set. A tuple $X \in K(n)$ is a **matrix extreme point** of the matrix convex set K if whenever it is represented as a proper matrix combination of the form (1.2) with $Y^\ell \in K(n_\ell)$, then $n = n_\ell$ and $X \overset{u}{\sim} Y^\ell$ for each ℓ. (We use $A \overset{u}{\sim} B$ to denote A and B are unitarily equivalent.) A tuple $X \in K(n)$ is an **absolute extreme point** (a *boundary point* in the terminology of [Kls14]) of K if whenever it is represented as a weakly proper

matrix combination of the form (1.2), then for each j either $n_j \leq n$ and $X \overset{u}{\sim} Y^j$ (and hence $n_j = n$), or $n_j > n$ and there exists a $Z^j \in K$ such that $Y^j \overset{u}{\sim} X \oplus Z^j$.

There is a different, dilation-theoretic viewpoint of matrix extreme points. Given a g-tuple α of $n \times m$ matrices and $\beta \in \mathbb{S}_m^g$, let

$$(1.3) \qquad\qquad Z = \begin{pmatrix} X & \alpha \\ \alpha^* & \beta \end{pmatrix}.$$

As a canonical geometric notion of an Arveson boundary representation, we say X is an **Arveson boundary point** of K if and only if $Z \in K(n+m)$ implies $\alpha = 0$. The tuple Z is n-**block diagonalizable** provided there exists a k, integers $n_j \leq n$ and tuples $E^j \in \mathbb{S}_{n_j}^g$ such that $Z \overset{u}{\sim} E^1 \oplus E^2 \oplus \cdots \oplus E^k$.

Our main general theorem is as follows.

Theorem 1.1. *Suppose K is a fully free set, n is a positive integer and $X \in K(n)$.*

(1) *X is a Euclidean extreme point of $K(n)$ if and only if, if $\alpha, \beta \in \mathbb{S}_n^g$ and Z as in equation (1.3) is in $K(2n)$, then $\alpha = 0$;*
(2) *X is a matrix extreme point of K if and only if X is irreducible and for each positive integer m, g-tuple α of $n \times m$ matrices and tuple $\beta \in \mathbb{S}_m^g$ if Z is in $K(n+m)$ and is n-block diagonalizable, then $\alpha = 0$;*
(3) *X is an absolute extreme point of K if and only if X is irreducible and in the Arveson boundary of K.*

The definition here of an Arveson boundary point for a free set mirrors the geometric formulation of a (not necessarily irreducible) boundary representation [Arv69] used by a number of authors including [Ag88, MS98, DM05, Arv08]. Item (3) explicitly connects, in the setting of $\mathbb{S}^g$, Kleski's notion of boundary point for a matrix convex set with that of an Arveson boundary point.

Theorem 1.1 makes clear the implications, Arveson boundary implies matrix extreme implies Euclidean extreme. Item (1) falls out of the usual argument that if K is matrix convex, then each $K(n)$ is convex. It is stated and proved as Proposition 2.1. Items (2) and (3) are stated and proved as Theorems 4.1 and 3.10 respectively.

1.3. **Free spectrahedra and polar duals.** A simple class of matrix convex sets is the solution sets of linear matrix inequalities (LMIs). Given a g-tuple $A \in \mathbb{S}^g$, let Λ_A denote the **homogeneous linear pencil**

$$\Lambda_A(x) = A_1 x_1 + \cdots + A_g x_g,$$

and L_A the **monic linear pencil**

$$L_A(x) = I - A_1 x_1 - \cdots - A_g x_g.$$

The corresponding **free spectrahedron** $\mathcal{D}_A = \big(\mathcal{D}_A(n)\big)_n$ is the sequence of sets

$$\mathcal{D}_A(n) = \{X \in \mathbb{S}_n^g \mid L_A(X) \succeq 0\}.$$

It is routine to verify that a free spectrahedron is matrix convex. Thus free spectrahedra are matrix convex subsets of $\mathbb{S}^g$ satisfying a finiteness condition. Conversely, as a special case of the Effros-Winkler matricial Hahn-Banach Theorem [EW97], if $K \subseteq \mathbb{S}^g$ is compact matrix convex and $0 \in K(1)$, then K is the (possibly infinite) intersection of free spectrahedra.

If $\Omega \in \mathbb{S}_d^g$ we say Ω has **size** d. A tuple B is a defining tuple for $\mathcal{D}_A$ if $\mathcal{D}_B = \mathcal{D}_A$ and Ω is a **minimal defining tuple** if Ω has minimal size among all defining tuples. The Gleichstellensatz [HKM13, Corollary 3.18 or Theorem 3.12] (see also [Zal17]) says any two minimal defining tuples for $\mathcal{D}_A$ are unitarily equivalent.

By analogy with the classical notion, the **free polar dual** $K^\circ = (K^\circ(n))_n$ of a free set $K \subseteq \mathbb{S}^g$ is

$$K^\circ(n) := \Big\{A \in \mathbb{S}_n^g : \ L_A(X) = I \otimes I - \sum_j^g A_j \otimes X_j \succeq 0 \text{ for all } X \in K\Big\}.$$

Note that the (free) polar dual of a matrix convex set is closed and matrix convex. We refer the reader to [EW97, HKM+] for basic properties of polar duals.

We do not know conditions on a closed matrix convex set K equivalent to the condition that K is the closed matrix convex hull of its Arveson boundary points. However, with a finiteness hypothesis Theorem 1.2, inspired by [Kls14, Corollary 2.4], gives an answer.

Theorem 1.2. *Suppose K is a closed matrix convex set containing 0. If $K^\circ = \mathcal{D}_\Omega$ and Ω is a minimal defining tuple for $\mathcal{D}_\Omega$, then there exists an N and irreducible tuples $\Omega^1, \ldots, \Omega^N$ in the Arveson boundary of K such that $\Omega = \oplus \Omega^j$ and*

(1.4) $$K = \mathrm{co}^{\mathrm{mat}}(\{\Omega\}) = \mathrm{co}^{\mathrm{mat}}(\{\Omega^1, \ldots, \Omega^N\}).$$

(Here $\mathrm{co}^{\mathrm{mat}}(\Gamma)$ denotes the matrix convex hull of $\Gamma \subseteq \mathbb{S}^g$, i.e., the smallest matrix convex set containing Γ.) Conversely, if there exists a tuple Ω such that (1.4) holds, then $K^\circ = \mathcal{D}_\Omega$.

Theorem 1.2 is proved in Section 5.

The theory of extreme points can be used to obtain properties of several basic spectrahedra. For example, in Section 7 we use it to deduce the following.

Corollary 1.3. *Let $A \in \mathbb{S}_d^g$. If the polar dual of $\mathcal{D}_A$ is again a free spectrahedron, then $\mathcal{D}_A(1)$ is a polyhedron. In particular, if $\mathcal{D}_A(1)$ is a ball, then $\mathcal{D}_A^\circ$ is not a free spectrahedron.*

Corollary 1.3 implies finitely generated matrix convex sets are rarely free spectrahedra. However, they are **free spectrahedrops**, i.e., projections of free spectrahedra [HKM+]. On the other hand, if K is a compact matrix convex free semialgebraic set containing 0 in its interior, then K is a free spectrahedron [HM12].

1.4. **Reader's Guide.** The rest of the paper is organized as follows. Section 2 recalls the classical notion of an extreme point in $\mathbb{R}^g$ and characterizes those for matrix convex sets (Proposition 2.1) and free spectrahedra (Corollary 2.3). Section 3 gives our first main result, Theorem 3.10 showing that an absolute extreme point is exactly an irreducible Arveson boundary point. In Section 4 we prove our second main result, a dilation theoretic characterization of matrix extreme points via the block-Arveson boundary, see Theorem 4.1. Section 5 gives the proof of our final main result: the polar dual of a matrix convex set is spanned by its finitely many Arveson boundary points if and only if it is a free spectrahedron (Theorem 1.2). We show the polar dual of a free spectrahedron is seldom a free spectrahedron in Corollary 6.3, and show it is one for a free simplex (Corollary 6.8). The paper concludes with Section 7 providing further applications and examples of matrix extreme points. The sets of extreme points for two types of matrix convex sets above the unit disk in $\mathbb{R}^2$ are studied in Subsection 7.2, where the Arveson boundary of the spin disk is identified and shown to span. Finally, in Subsection 7.3 the matrix convex hull of the TV screen is investigated.

2. Euclidean (Classical) Extreme Points

In this section we establish Theorem 1.1 (1) characterizing Euclidean extreme points of fully free sets. This characterization reduces to a result of Ramana-Goldman [RG95] in the case K is a free spectrahedron, see Corollary 2.3.

Recall, a point v of a convex set $C \subseteq \mathbb{R}^g$ is an **(Euclidean) extreme point** of C, in the classical sense, if $v = \lambda a + (1 - \lambda)b$ for $a, b \in C$ and $0 < \lambda < 1$ implies $a = v = b$. Let $\partial^{\mathrm{Euc}}C$ denote its set of Euclidean extreme points. Note that this definition makes sense even if C is not assumed convex.

While the interest here is in matrix convex sets K such as free spectrahedra, it is of course natural to consider, for fixed n, the extreme points of the convex set $K(n) \subseteq \mathbb{S}_n^g$. The next result is a dilation style characterization of Euclidean extreme points of $K(n)$.

Proposition 2.1. *Suppose Γ is a fully free set, n is a positive integer and $X \in \Gamma(n)$. If X is a Euclidean extreme point of $\Gamma(n)$, $\alpha \in \mathbb{S}_n^g$ and*

$$\begin{pmatrix} X & \alpha \\ \alpha & X \end{pmatrix} \in K(2n),$$

then $\alpha = 0$. Conversely, if X is not an extreme point, then there exists $0 \neq \alpha \in \mathbb{S}_n^g$ with

$$(2.1) \qquad\qquad W = \begin{pmatrix} X & \alpha \\ \alpha & X \end{pmatrix} \in K(2n).$$

Finally, if Γ is matrix convex, X is a Euclidean extreme point and for some $\alpha \in (\mathbb{C}^{n \times n})^g$ we have

$$(2.2) \qquad\qquad Z = \begin{pmatrix} X & \alpha^* \\ \alpha & X \end{pmatrix} \in \Gamma(2n),$$

it follows that $\alpha = 0$.

Proof. Suppose $X \in \Gamma(n)$ is not a Euclidean extreme point for $\Gamma(n)$. Thus, there exists a $0 \neq \alpha \in \mathbb{S}_n^g$ such that $X \pm \alpha \in \Gamma(n)$. Since Γ is closed with respect to direct sums, $Y = (X + \alpha) \oplus (X - \alpha) \in \Gamma(2n)$. Let U denote the $2n \times 2n$ unitary matrix

(2.3)
$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} I_n & -I_n \\ I_n & I_n \end{pmatrix}$$

Since Γ is closed with respect to unitary similarity,

$$U^* Y U = \begin{pmatrix} X & \alpha \\ \alpha & X \end{pmatrix} \in \Gamma(2n).$$

To prove the converse suppose $X \in \Gamma(n)$ is a Euclidean extreme point, $\alpha \in \mathbb{S}_n^g$ and W is as in equation (2.1). With U as in equation (2.3), we have

$$UWU^* = \begin{pmatrix} X + \alpha & 0 \\ 0 & X - \alpha \end{pmatrix} \in \Gamma(2n).$$

Since Γ is fully free, both $X \pm \alpha \in \Gamma(n)$. Thus, $X = \frac{1}{2}[(X + \alpha) + (X - \alpha)]$. Since X is an extreme point, $X + \alpha = X$; i.e., $\alpha = 0$.

Finally, suppose Γ is matrix convex and Z is as in equation (2.2). Let

$$F = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad G = \begin{pmatrix} iI & 0 \\ 0 & I \end{pmatrix}.$$

Since

$$\frac{1}{2}(F^* Z F + Z) = \begin{pmatrix} X & \gamma \\ \gamma & X \end{pmatrix},$$

where $\gamma = \frac{1}{2}(\alpha + \alpha^*)$, it follows from what has already been proved that $\alpha + \alpha^* = 0$. On the other hand,

$$\frac{1}{2}(G^* Z G + G F^* Z F G^*) = \begin{pmatrix} X & \delta \\ \delta & X \end{pmatrix} \in \Gamma(2n),$$

where $\delta = \frac{1}{2}(-i\alpha + i\alpha^*) = \frac{i}{2}(\alpha^* - \alpha)$. Thus, again by what has already been proved, $\alpha - \alpha^* = 0$. Hence $\alpha = 0$. ∎

We next consider, for fixed n, the extreme points of the spectrahedron $\mathcal{D}_A(n) \subseteq \mathbb{S}_n^g$ and this was done by Ramana and Goldman [RG95] for $n = 1$. Below is a sample result.

Theorem 2.2 (Ramana and Goldman [RG95, Corollary 3]). *Fix $A \in \mathbb{S}_d^g$. A point $X \in \mathcal{D}_A(1)$ is an Euclidean extreme point of $\mathcal{D}_A(1)$ if and only if $Y \in \mathbb{R}^g$ and $\ker L_A(X) \subseteq \ker \Lambda_A(Y)$ implies $Y = 0$.*

The next corollary is an immediate consequence of Proposition 2.1 and the proof of Theorem 2.2.

Corollary 2.3. *For a point $X \in \mathcal{D}_A(n)$ the following are equivalent.*

(i) X is an Euclidean extreme point of $\mathcal{D}_A(n)$;

(ii) $Y \in \mathbb{S}_n^g$ and $\ker L_A(X) \subseteq \ker \Lambda_A(Y)$ implies $Y = 0$;

(iii) $W \in \mathcal{D}_A(n)$ and $\ker L_A(X) \subseteq \ker L_A(W)$ implies $\ker L_A(X) = \ker L_A(W)$;

(iv) $\alpha, \beta \in \mathbb{S}_n^g$ and

$$Z = \begin{pmatrix} X & \alpha \\ \alpha & \beta \end{pmatrix} \in \mathcal{D}_A(2n)$$

implies $\alpha = 0$.

Proof. The proof uses the following observation. If $L(X) \succeq 0$ and $Y \in \mathbb{S}_n^g \setminus \{0\}$ satisfies $\ker L(X) \subseteq \ker \Lambda(Y)$, then there exists a $t \in \mathbb{R}$ such that $L(X \pm tY) \succeq 0$ and the kernel of $L(X + tY)$ strictly contains the kernel of $L(X)$. To prove this assertion, simply note that $L(X \pm tY) = L(X) \pm t\Lambda(Y)$ and the hypotheses imply that the range of the self-adjoint matrix $\Lambda(Y)$ lies inside the range of the positive semidefinite matrix $L(X)$.

Theorem 2.2 gives the equivalence of items (i) and (ii) in the case $n = 1$, but their proof adapts easily to general n. A proof is included here for the readers convenience. If X is an extreme point of $\mathcal{D}_A$, and $\ker L_A(X) \subseteq \Lambda_A(Y)$, then choosing t as above, gives $L_A(X \pm tY) \succeq 0$. Hence $X \pm tY \in \mathcal{D}_A$ and therefore $Y = 0$. Hence item (i) implies item (ii). Conversely, if X is not an extreme point of $\mathcal{D}_A$, then there exists a non-zero Y such that $X \pm Y \in \mathcal{D}_A$. In particular, $0 \preceq L_A(X + Y) = L_A(X) \pm \Lambda_A(Y)$ and hence $\ker \Lambda(Y) \supseteq \ker L_A(X)$. Hence item (i) and item (ii) are equivalent.

Suppose $Y \neq 0$ and $\ker L_A(X) \subseteq \Lambda_A(Y)$. By the observation at the outset of the proof, there is a $t \neq 0$ such that

$$0 \preceq L_A(X \pm tY) = L_A(X) \pm t\Lambda_A(Y).$$

and the kernel of $L_A(X + tY)$ strictly contains that of $L_A(X)$. Hence item (iii) implies item (ii). On the other hand, if $\ker L_A(X) \subseteq \ker L_A(W)$, then with $Y = X - W$, the kernel of $L_A(X)$ is contained in the kernel of $\Lambda_A(Y)$. In particular, if (ii) holds, then $Y = 0$ and hence $W = X$. Thus $\ker L_A(X) = \ker L_A(W)$ and item (ii) implies item (iii).

That item (iv) implies item (i) is seen by taking $\beta = X$ and applying Proposition 2.1. Now suppose item (ii) holds and Z is given as in item (iv). By considering $L_A(Z)$, it follows that $\ker(L_A(X)) \subseteq \ker(\Lambda_A(\alpha))$. Hence $\alpha = 0$. ∎

3. ARVESON BOUNDARY AND ABSOLUTE EXTREME POINTS

Now we turn to Arveson boundary points and absolute extreme points (*boundary points* in the terminology of [Kls14]) of a free set as defined in the introduction. We shall establish Theorem 1.1 (3), see Theorem 3.10, showing that absolute extreme points are exactly irreducible Arveson boundary points.

3.1. **Matrix convex hulls.** In this subsection we describe the matrix convex hull of an arbitrary subset $\Gamma \subseteq \mathbb{S}^g$.

The **matrix convex hull** of an arbitrary subset $\Gamma \subseteq \mathbb{S}^g$ is defined to be the intersection of all matrix convex sets containing Γ. It is easily seen to be convex and is thus the smallest matrix convex set that contains Γ. Let $K = \mathrm{co}^{\mathrm{mat}}(\Gamma)$ denote the matrix convex hull of Γ and $\overline{\mathrm{co}}^{\mathrm{mat}}(\Gamma)$ the **closed matrix convex hull** of Γ obtained by taking the ordinary (in $\mathbb{S}_n^g$) closures of each $K(n)$. A routine exercise shows $\mathrm{co}^{\mathrm{mat}}(\Gamma)$ is matrix convex and is thus the smallest closed matrix convex set containing Γ. As an example, each $\Omega \in \mathbb{S}^g$ gives rise to the **finitely generated** matrix convex set,

$$(3.1) \qquad \mathrm{co}^{\mathrm{mat}}(\{\Omega\}) = \big\{ V^*(I_m \otimes \Omega)V : m \in \mathbb{N}, \ V \text{ is an isometry} \big\}.$$

Proposition 3.1. *A point $X \in \mathbb{S}_n^g$ is in the matrix convex hull of the free set Γ if and only if there is a positive integer N, a tuple $Z \in \Gamma(N)$ and an isometry $V : \mathbb{C}^n \to \mathbb{C}^N$ such that $X = V^*ZV$.*

Proof. For positive integers n, let $K(n)$ denote those $n \times n$ tuples X for which there exits a positive integer N, an isometry $V : \mathbb{C}^n \to \mathbb{C}^N$ and a tuple $Z \in \Gamma(N)$ such that $X = V^*ZV$. Since Γ is closed with respect to direct sums, so is $K = (K(n))_n$. Suppose now $W : \mathbb{C}^\ell \to \mathbb{C}^n$ is an isometry. Let Y denote the isometry $Y : \mathbb{C}^\ell \to \mathbb{C}^N$ given by $Y = VW$. It follows that

$$Y^*ZY = W^*XW.$$

Since $Z \in \Gamma(N)$, by definition $W^*XW \in K(\ell)$. Hence K is closed with respect to isometric conjugation and is therefore a matrix convex set. ∎

Remark 3.2. If $\Gamma \subseteq \mathbb{S}^g$ is a finite set, then Theorem 1.2 implies $\mathrm{co}^{\mathrm{mat}}(\Gamma)$ is closed. (It is not hard to give a direct proof of this fact.) At least as far as we are aware for a compact set $\Gamma \subseteq \mathbb{S}_n^g$, its matrix convex hull $\mathrm{co}^{\mathrm{mat}}(\Gamma)$ is not necessarily closed. Thus $\overline{\mathrm{co}}^{\mathrm{mat}}(\Gamma)$ is potentially larger than $\mathrm{co}^{\mathrm{mat}}(\Gamma)$.

3.2. **Arveson boundary.** In this subsection we recall the notion of the Arveson boundary of a free set and develop some of its basic properties.

Given a free set Γ and a positive integer n, a tuple $X \in \Gamma(n)$ is in the the **Arveson boundary of Γ** or is an **Arveson boundary point** of Γ, written $X \in \partial^{\mathrm{arv}}\Gamma$, if given a positive integer m and g-tuples α of size $n \times m$ and β of size $m \times m$ such that

$$(3.2) \qquad \begin{pmatrix} X & \alpha \\ \alpha^* & \beta \end{pmatrix} \in \Gamma(n+m)$$

it follows that $\alpha = 0$. A coordinate free definition is as follows. The point $\Gamma \in K(n)$ is an Arveson boundary point of K if for each m each Y in $K(m)$ and isometry $V : \mathbb{C}^n \to \mathbb{C}^m$ such that $X = V^*YV$ it follows that $VX = YV$.

The following statement is a simple consequence of Proposition 2.1.

Proposition 3.3. *Suppose Γ is a free set and n is a positive integer. If $X \in \Gamma(n)$ is an Arveson boundary point for Γ, then X is a Euclidean extreme point of $\Gamma(n)$.*

The next lemma says for a matrix convex set the property (3.2) in the definition of an Arveson boundary point only needs to be verified for column tuples α.

Lemma 3.4. *Suppose K is matrix convex and*

$$Z = \begin{pmatrix} X & \alpha \\ \alpha^* & \beta \end{pmatrix} \in K(m + \ell).$$

If $v \in \mathbb{R}^\ell$ is a unit vector, then

$$Y = \begin{pmatrix} X & \alpha v \\ v^*\alpha^* & v^*\beta v \end{pmatrix} \in K(m + 1).$$

Proof. Consider the isometry

$$W = \begin{pmatrix} I_n & 0 \\ 0 & v \end{pmatrix}.$$

Since K is matrix convex,

$$W^* Z W = Y \in K(m + 1). \qquad \blacksquare$$

Lemma 3.5. *Suppose $\Gamma \subseteq \mathbb{S}^g$ is matrix convex. A tuple $X \in \mathbb{S}_n^g$ is in the Arveson boundary of Γ if and only if, given a g-tuple α from $\mathbb{C}^n$ and $\beta \in \mathbb{C}^g$ such that*

$$\begin{pmatrix} X & \alpha \\ \alpha^* & \beta \end{pmatrix} \in \Gamma$$

it follows that $\alpha = 0$.

Proof. Apply Lemma 3.4. $\qquad \blacksquare$

Lemma 3.6. *If $\Gamma \subseteq \mathbb{S}^g$ is a free set, then the Arveson boundary of Γ is closed with respect to direct sums and unitary similarity; i.e., it is a free set.*

Proof. The proof regarding unitary conjugation is trivial. Onward to direct sums. Suppose X, Y are both in the Arveson boundary and

(3.3)
$$Z := \begin{pmatrix} X & 0 & B_{11} & B_{12} \\ 0 & Y & B_{21} & B_{22} \\ B_{11} & B_{21}^* & D_{11} & D_{12} \\ B_{12}^* & B_{22}^* & D_{12}^* & D_{22} \end{pmatrix}$$

is in Γ. Writing Z as

$$\begin{pmatrix} X & \begin{pmatrix} 0 & B_{11} & B_{12} \end{pmatrix} \\ \begin{pmatrix} 0 \\ B_{11}^* \\ B_{12}^* \end{pmatrix} & \begin{pmatrix} Y & B_{21} & B_{22} \\ B_{21}^* & D_{11} & D_{12} \\ B_{22}^* & D_{12}^* & D_{22} \end{pmatrix} \end{pmatrix} \in \Gamma$$

and using the assumption that $X \in \partial^{\mathrm{arv}}\Gamma$ it follows that $B_{11} = 0$ and $B_{12} = 0$. Reversing the roles of X and Y shows $B_{21} = 0$ and $B_{22} = 0$. ∎

Proposition 3.7. *If Γ is a fully free set, then $\partial^{\mathrm{arv}}\Gamma = \partial^{\mathrm{arv}}\mathrm{co}^{\mathrm{mat}}\Gamma$.*

Lemma 3.8. *If $\Gamma \subseteq \Gamma' \subseteq \mathbb{S}^g$ and $X \in \Gamma$ is an Arveson boundary point of Γ', then X is an Arveson boundary point of Γ.*

Proof. Evident. ∎

Proof of Proposition 3.7. Suppose A is in $\partial^{\mathrm{arv}}\mathrm{co}^{\mathrm{mat}}\Gamma$. Since A is in $\mathrm{co}^{\mathrm{mat}}\Gamma$, by Proposition 3.1 there exists an X in Γ of the form

$$X = \begin{pmatrix} A & B \\ B^* & C \end{pmatrix}.$$

Since $X \in \mathrm{co}^{\mathrm{mat}}\Gamma$ and A is an Arveson boundary point of $\mathrm{co}^{\mathrm{mat}}\Gamma$, it follows that $B = 0$. Since Γ is closed with respect to restrictions to reducing subspaces, $A \in \Gamma$. By Lemma 3.8, $A \in \partial^{\mathrm{arv}}\Gamma$.

For the converse, suppose $A \in \partial^{\mathrm{arv}}\Gamma$ and let α, W such that $\alpha \neq 0$ such that

$$Z = \begin{pmatrix} A & \alpha \\ \alpha^* & W \end{pmatrix} \in \mathrm{co}^{\mathrm{mat}}\Gamma$$

be given. By Proposition 3.1, there is a dilation X of Z lying in Γ; i.e., there exists δ, γ, Y such that

$$(3.4) \qquad\qquad X = \begin{pmatrix} A & \alpha & \gamma \\ \alpha^* & W & \delta \\ \gamma^* & \delta^* & Y \end{pmatrix} \in \Gamma.$$

Since $A \in \partial^{\mathrm{arv}}\Gamma$ and $X \in \Gamma$, it follows that $\alpha = 0$. Hence $A \in \partial^{\mathrm{arv}}\mathrm{co}^{\mathrm{mat}}(\Gamma)$. ∎

Remark 3.9. Assuming Γ is compact, we do not know if Proposition 3.7 holds with $\partial^{\mathrm{arv}}\mathrm{co}^{\mathrm{mat}}\Gamma$ replaced by $\partial^{\mathrm{arv}}\overline{\mathrm{co}}^{\mathrm{mat}}\Gamma$ a statement equivalent to $\partial^{\mathrm{arv}}\mathrm{co}^{\mathrm{mat}}\Gamma = \partial^{\mathrm{arv}}\overline{\mathrm{co}}^{\mathrm{mat}}\Gamma$.

3.3. Absolute extreme points vs. Arveson boundary.

The tuple $X \in \mathbb{S}^g$ is **irreducible** if there does not exist a nontrivial common invariant subspace for the set $\{X_1, \ldots, X_g\}$. Observe invariant equals reducing since the matrices X_j are self-adjoint.

Theorem 3.10. *Suppose K is a fully free set. A point $X \in K$ is an absolute extreme point of K if and only if X is irreducible and in the Arveson boundary of K.*

The fact that an absolute extreme point is irreducible is rather routine. For completeness, we include a proof.

Lemma 3.11. *Suppose $K \subseteq \mathbb{S}^g$ is a fully free set. If $X \in K$ is either a matrix extreme point or an absolute extreme point of K, then X is irreducible.*

Proof. Suppose $X \in K(n)$ is a matrix extreme point of K. If X is not irreducible, then there exists nontrivial reducible subspaces H_1 and H_2 for the set $\{X_1, \ldots, X_g\}$ such that $\mathbb{C}^n = H_1 \oplus H_2$. Let $V_\ell : H_\ell \to \mathbb{C}^n$ denote the inclusion mappings. Let $Y^\ell = V_\ell V_\ell^* X V_\ell V_\ell^*$. Since K is closed with respect to reducing subspaces, $Y^\ell \in K$ and moreover the mappings $V_\ell V_\ell^*$ are proper. Evidently,

$$X = \sum V_\ell^* Y^\ell V_\ell.$$

Since this sum is a proper combination from K, we have that X and Y^ℓ are unitarily equivalent, a contradiction since the size of X strictly exceeds that of Y_ℓ. If X is an absolute extreme point, then X is a matrix extreme point and hence is irreducible by what has already been proved. ∎

3.3.1. *A non-interlacing property.* In this subsection we present a lemma on an interlacing property we will use in the proofs of Theorems 3.10 and 1.2; cf. Cauchy's interlacing theorem [HJ12, Theorem 4.3.8].

Lemma 3.12. *Let D denote the $n \times n$ diagonal matrix with diagonal entries $\lambda_1, \ldots, \lambda_n \in \mathbb{C}$ and let*

$$E = \begin{pmatrix} D & a \\ a^* & e \end{pmatrix}.$$

If $f \in \mathbb{C}$ and E is unitarily equivalent to

$$F = \begin{pmatrix} D & 0 \\ 0 & f \end{pmatrix},$$

then $a = 0$.

Proof. Denote the entries of a by $a_1, \ldots, a_n$. By induction,

$$\det(E - tI) = p(t)(e - t) - \sum a_j^2 \prod_{k \neq j} (\lambda_k - t),$$

where $p(t) = \prod(\lambda_k - t)$. On the other hand, $\det(F - tI) = p(t)(f - t)$. Thus,

$$p(t)(e - f) = p(t)(e - t) - p(t)(f - t) = \sum a_j^2 \prod_{k \neq j} (\lambda_k - t).$$

The left hand side is 0 or has degree n in t; whereas the right hand side is either 0 or has degree $n - 1$ in t. The conclusion is that both sides are 0 and thus $a_j = 0$ and $e = f$. Here we have used in a very strong way that the matrices E and F are each self-adjoint (in which case unitary equivalence is the same as similarity). ∎

Lemma 3.13. *Suppose $K \subseteq \mathbb{S}^g$ is free set and n is a positive integer. If $X \in K(n)$ is an absolute extreme point of K and if α is a g-tuple from $\mathbb{C}^n$, $\beta \in \mathbb{R}^g$ and*

$$Y = \begin{pmatrix} X & \alpha \\ \alpha^* & \beta \end{pmatrix} \in K(n+1)$$

then $\alpha = 0$.

Proof. Letting $V : \mathbb{C}^n \to \mathbb{C}^{n+1} = \mathbb{C}^n \oplus \mathbb{C}$ denote the isometry $Vx = x \oplus 0$, observe $X = V^*YV$. Using the definition of absolute extreme point, it follows that there is a $\gamma \in \mathbb{C}$ such that

$$Y \overset{u}{\sim} Z = \begin{pmatrix} X & 0 \\ 0 & \gamma \end{pmatrix}.$$

By Lemma 3.12, $\alpha = 0$ and the proof is complete. ∎

3.4. **Proof of Theorem 3.10.** For the proof of the forward direction of Theorem 3.10, suppose X is an absolute extreme point. Lemmas 3.11 and 3.13 together with Lemma 3.5 show X is irreducible and an Arveson boundary point respectively.

The proof of the reverse direction of Theorem 3.10 uses the following lemma.

Lemma 3.14. *Fix positive integer n and m and suppose C is a nonzero $m \times n$ matrix, the tuple $X \in \mathbb{S}_n^g$ is irreducible and $E \in \mathbb{S}_m^g$. If $CX_i = E_iC$ for each i, then C^*C is a nonzero multiple of the identity. Moreover, the range of C reduces the set $\{E_1, \ldots, E_g\}$ so that, up to unitary equivalence, $E = X \oplus Z$ for some $Z \in \mathbb{S}_k^g$, where $k = m - n$.*

Proof. To prove this statement note that

$$X_jC^* = C^*E_j.$$

It follows that

$$X_jC^*C = C^*E_jC = C^*CX_j.$$

Since $\{X_1, \ldots, X_g\}$ is irreducible, C^*C is a nonzero multiple of the identity and therefore C is a multiple of an isometry. Further, since $CX = EC$, the range of C is invariant for E. Since each E_j is self-adjoint, the range of C reduces each E_j and C, as a mapping into its range is a multiple of a unitary. ∎

To complete the proof of the reverse direction, suppose X is both irreducible and in the Arveson boundary of K. To prove X is an absolute extreme point, suppose

$$X = \sum_{j=1}^{\nu} C_j^* E^j C_j,$$

where each C_j is nonzero, $\sum_{j=1}^{\nu} C_j^*C_j = I$ and $E_j \in K$. In this case, let

$$C = \begin{pmatrix} C_1 \\ \vdots \\ C_\nu \end{pmatrix} \quad \text{and} \quad E = E^1 \oplus E^2 \oplus \cdots \oplus E^\nu$$

and observe that C is an isometry and $X = C^*EC$. Hence, as X is in the Arveson boundary, $CX = EC$. It follows that $C_jX_k = E_k^jC_j$ for each j and k. Thus, by Lemma 3.14, it follows that each E_j is unitarily equivalent to $X \oplus Z^j$ for some $Z^j \in K$. Thus X is an absolute extreme point. ∎

4. Matrix Extreme Points and the Block-Arveson Boundary

In this section we turn our attention to matrix extreme points and the block-Arveson boundary. Theorem 4.1 is the main result of this section. It gives an Arveson-type dilation characterization of matrix extreme points.

We say the tuple $X \in K(n)$ is in the **block-Arveson boundary** or is a **block-Arveson boundary point** of a matrix convex set K if whenever

$$\begin{pmatrix} X & \alpha \\ \alpha^* & \beta \end{pmatrix} \in K$$

is n-block diagonalizable, $\alpha = 0$.

Theorem 4.1. *Let K be a matrix convex set. A point X is a matrix extreme point of K if and only if X is both irreducible and in the block-Arveson boundary of K.*

4.1. **Matrix extreme points.** We now recall the definition of matrix extreme points and the corresponding Krein-Milman theorem of Webster-Winkler [WW99].

The matrix convex combination (1.2) is **proper** provided each V_ℓ is surjective. Note that in this case, $n \geq n_\ell$ for each ℓ. A tuple $X \in K(n)$ is a **matrix extreme point** of the matrix convex set K if whenever it is represented as a proper matrix combination of the form (1.2) with $Y^\ell \in K(n_\ell)$, then $n = n_\ell$ and $X \overset{u}{\sim} Y_\ell$ for each ℓ. (Recall: we use $A \overset{u}{\sim} B$ to denote A and B are unitarily equivalent.) The set of all matrix extreme points will be denoted by $\partial^{\mathrm{mat}} K$. Webster-Winkler give in [WW99, Theorem 4.3] a Krein-Milman theorem in the matrix convex setting. (See also [Far00] for an alternate proof and the elucidating discussion of the connection between matrix extreme points of K and matrix states on an operator system.)

Theorem 4.2 (Webster-Winkler [WW99, Theorem 4.3])**.** *If $K \subseteq \mathbb{S}^g$ be a compact matrix convex set, then $\partial^{\mathrm{mat}} K$ is non-empty, and K is the smallest closed matrix convex set containing $\partial^{\mathrm{mat}} K$, i.e.,*

$$\overline{\mathrm{co}}^{\mathrm{mat}} \partial^{\mathrm{mat}} K = K.$$

Corollary 4.3. *Let K be a compact matrix convex set. Then K is the smallest closed matrix convex set containing the block-Arveson boundary of K.*

Proof. Simply combine Theorem 4.1 with Theorem 4.2. ∎

Remark 4.4. Suppose the matrix convex combination (1.2) is not necessarily proper. Let P_ℓ denote the inclusion of the range of Y^ℓ into $\mathbb{C}^{n_\ell}$ and let $Z^\ell = P_\ell^* Y^\ell P_\ell$. Likewise, let $W_\ell = P_\ell^* V_\ell$. With these choices,

$$X = \sum_\ell W_\ell^* Z^\ell W_\ell$$

is a proper matrix convex combination. Moreover, the set K is closed with respect to isometric similarity and if each $Y^\ell \in K(n_\ell)$, then this sum is a matrix convex combination from K.

The following lemma gives a convenient alternate definition of matrix extreme point in the setting of $\mathbb{S}^g$.

Lemma 4.5. *Suppose K is a matrix convex set, n is a positive integer and $X \in K(n)$. The point X is a matrix extreme point of K if and only if whenever X is represented as a convex combination as in equation* (1.2) *with $n_\ell \le n$ and $Y^\ell \in K(n_\ell)$ for each ℓ, then, for each ℓ, either $V_\ell = 0$ or $n_\ell = n$ and $Y^\ell \overset{u}{\sim} X$.*

Proof. First suppose X is a matrix extreme point of K and is represented as in equation (1.2) with $n_\ell \le n$ and $Y^\ell \in K(n_\ell)$ for each ℓ. In the notation of Remark 4.4, $Z^\ell \in K$ by matrix convexity and each W_ℓ is proper (or 0). Let $L = \{\ell : W_\ell \ne 0\}$. Thus,

$$X = \sum_{\ell \in L} W_\ell^* Z^\ell W_\ell$$

is a proper convex combination. Since X is matrix extreme $Z^\ell \overset{u}{\sim} X$ and therefore the range of W_ℓ (equal the range of V_ℓ) is n. Since $n_\ell \le n$, it follows that for each ℓ either $V_\ell = 0$ or V_ℓ is proper and $Y^\ell \overset{u}{\sim} X$.

To prove the converse fix $X \in K(n)$ and suppose whenever X is represented in as a matrix convex combination as in equation (1.2) with $n_\ell \le n$ and $Y^\ell \in K(n_\ell)$, then either $V^\ell = 0$ or $n_\ell = n$ and $Y^\ell \overset{u}{\sim} X$. To prove X is a matrix extreme point of K, suppose X is represented as a matrix convex combination as in equation (1.2) and each V_ℓ is surjective. In particular, $n_\ell \le n$. Since $V_\ell \ne 0$, it follows that $Y^\ell \overset{u}{\sim} X$ for each ℓ and therefore X is a matrix extreme point of K. ∎

4.2. **Points which are convex combinations of themselves.** Before turning to the proof of Theorem 4.1, we present an intermediate result of independent interest.

Proposition 4.6. *Suppose X is a tuple of size N and $C_1, \dots, C_t$ are $N \times N$ matrices. If*

(i) $X \in \mathbb{S}^g_n$ *is irreducible;*

(ii) $X = \sum_{\ell=1}^t C_\ell^* X C_\ell$;

(iii) $\sum C_\ell^* C_\ell = I$,

then each C_ℓ is a scalar multiple of the identity.

Proof. Consider the completely positive map $\phi : M_N(\mathbb{C}) \to M_N(\mathbb{C})$ given by

$$A \mapsto \sum_{j=1}^t C_j^* A C_j.$$

Since X_j are fixed points of ϕ and they generate $M_N(\mathbb{C})$ by irreducibility, Arveson's [Arv72, Boundary Theorem 2.1.1] (cf. [Arv72, Remark 2, p. 288]) implies that ϕ is the identity map. The Unitary freedom in a Choi-Kraus representation (see e.g. [NC10, Theorem 8.2]) now concludes the proof. ∎

We next give an alternative proof of Proposition 4.6 based on the theory of linear matrix inequalities and free spectrahedra.

Lemma 4.7. *Let $X \in \mathbb{S}_N^g$ be given. For $S \in \mathbb{S}_N^g$, let Γ_S denote the eigenspace corresponding to the largest eigenvalue λ_S of $\Lambda_X(S)$.*

If X is irreducible and if C is an $N \times N$ matrix such that $(C \otimes I_N)\Gamma_S \subseteq \Gamma_S$ for all $S \in \mathbb{S}_N^g$, then C is a multiple of the identity.

Lemma 4.8. *Suppose $X, Y \in \mathbb{S}^g$ and $n \in \mathbb{N}$. If $\mathcal{D}_X(n) \subseteq \mathcal{D}_Y(n)$ and $\partial\mathcal{D}_X(n) \subseteq \partial\mathcal{D}_Y(n)$, then $\mathcal{D}_X(n) = \mathcal{D}_Y(n)$.*

If $N \geq M$, $X \in \mathbb{S}_N^g$ and $Y \in \mathbb{S}_M^g$ and if $\mathcal{D}_X(N) = \mathcal{D}_Y(N)$, then $\mathcal{D}_X = \mathcal{D}_Y$.

Proof. Suppose $T \in \mathcal{D}_Y(n) \setminus \mathcal{D}_X(n)$. Since $\mathcal{D}_X(n)$ is convex and contains 0 in its interior, there is a $0 < t < 1$ such that $tT \in \partial\mathcal{D}_X(n)$. Hence $tT \in \partial\mathcal{D}_Y(n)$, a contradiction (because $\mathcal{D}_Y(n)$ is also convex and contains 0 in its interior).

Now suppose $N \geq M$, $X \in \mathbb{S}_N^g$ and $Y \in \mathbb{S}_M^g$ and $\mathcal{D}_X(N) = \mathcal{D}_Y(N)$. First observe, if $m \leq N$, then $\mathcal{D}_X(m) = \mathcal{D}_Y(m)$. Now let $n \in \mathbb{N}$, $S \in \mathcal{D}_X(n)$ and a vector $\gamma \in \mathbb{C}^M \otimes \mathbb{C}^n$ be given. Write

$$\gamma = \sum_{j=1}^{M} e_j \otimes \gamma_j \in \mathbb{C}^M \otimes \mathbb{C}^n.$$

Let $\mathcal{W}$ denote the span of $\{\gamma_j : 1 \leq j \leq M\}$ and let $W : \mathcal{W} \to \mathbb{C}^n$ denote the inclusion. Finally, let $T = W^*SW$. It follows that the size m of T is at most N and $T \in \mathcal{D}_X(m)$. Hence $T \in \mathcal{D}_Y(m)$ and therefore,

$$0 \leq \langle (I - \Lambda_Y(T))\gamma, \gamma \rangle = \langle (I - \Lambda_Y(S))\gamma, \gamma \rangle.$$

So $S \in \mathcal{D}_Y(n)$. Thus $\mathcal{D}_X \subseteq \mathcal{D}_Y$ and thus, by symmetry, $\mathcal{D}_X = \mathcal{D}_Y$. ∎

Proof of Lemma 4.7. Since Γ_S is invariant under $C \otimes I$, there is a an eigenvector $\gamma \in \Gamma_S$ for $C \otimes I$. (Such eigenvectors exist and we note that this is the only place where complex, as opposed to real, scalars are used.) In particular, letting Δ_j denote the eigenspaces for C, for each S in $\mathbb{S}_N^g$ there is a j such that $(\Delta_j \otimes \mathbb{C}^N) \cap \Gamma_S \neq (0)$.

Let $V_j : \Delta_j \to \mathbb{C}^N$ denote the inclusion and let $Y^j = V_j^*XV_j$. Let $Y = \oplus_k Y^j$ (the orthogonal direct sum, even though the subspaces Δ_j might not be orthogonal). In particular, $Y \in \mathbb{S}_M^g$ for some $M \leq N$. Suppose $S \in \mathcal{D}_X(N)$. It follows that $S \in \mathcal{D}_{Y^j}$ for each j and hence $X \in \mathcal{D}_Y(N)$; i.e., $\mathcal{D}_X(N) \subseteq \mathcal{D}_Y(N)$. If $S \in \partial\mathcal{D}_X(N)$, then there is a j and vector

$0 \neq \gamma_j \in \Delta_j \otimes \mathbb{C}^N$ such that $(I - \Lambda_X(S))\gamma = 0$. Let γ' denote the corresponding vector in $\oplus_k \Delta_k$; i.e., $0 \neq \gamma' = \oplus_k \gamma'_k$ where $\gamma'_k = 0$ for $k \neq j$ and $\gamma'_j = \gamma \neq 0$. It follows that

$$(I - \Lambda_Y(S))\gamma' = \oplus_k(I - \Lambda_{Y^k}(S))\gamma'_k = (I - \Lambda_{Y^j}(S))\gamma'_j = (I - \Lambda_X(S))\gamma = 0.$$

Hence, $(I - \Lambda_Y(S))\gamma' = 0$ and therefore $S \in \partial \mathcal{D}_Y(N)$. Another application of Lemma 4.8 now implies $\mathcal{D}_X(N) = \mathcal{D}_Y(N)$. Lemma 4.8 implies $\mathcal{D}_X = \mathcal{D}_Y$. Assuming X is irreducible, it is a minimal defining tuple, cf. [HKM13, Proposition 3.17 or Corollary 3.18] (see also [Zal17]). On the other hand, the size of Y is at most that of X and thus, by the Gleichstellensatz [HKM13, Theorem 3.12], they (have the same size and) are unitarily equivalent. Since X is irreducible so is Y. Thus, as $Y = \oplus_k Y^k$, we conclude that there is only one summand, say Y^1. Moreover, C has only one eigenspace $\Delta_1 = \mathbb{C}^N$, so it is a multiple of the identity. ∎

Alternate Proof of Proposition 4.6. Let $S \in \mathbb{S}_N^g$ be given and fix $\gamma \in \Gamma_S$. As before, let λ_S denote the largest eigenvalue of $\Lambda_X(S)$ and let Γ_S denote the corresponding eigenspace. Note that

$$\lambda_S - \Lambda_X(S) = \sum_{\ell=1}^{t}(C_\ell^* \otimes I)(\lambda_S - \Lambda_X(S))(C_\ell \otimes I).$$

Observe $\lambda_S - \Lambda_X(S) \succeq 0$ and $(\lambda_S - \Lambda_X(S))\gamma = 0$ together imply that for each $1 \leq \ell \leq t$,

$$(C_\ell \otimes I)\gamma \in \Gamma_S.$$

Thus $(C_\ell \otimes I_N)\Gamma_S \subseteq \Gamma_S$ so that the subspaces Γ_S are all invariant under each $C_\ell \otimes I_N$. By Lemma 4.7 each C_ℓ is a multiple of the identity. ∎

4.3. **Proof of Theorem 4.1.** We are finally ready to prove Theorem 4.1. We isolate each of its two implications in a separate lemma.

Lemma 4.9. *Let X be a matrix tuple of size N. If X is matrix extreme in the matrix convex set K, then X is in the block-Arveson boundary of K.*

Proof. Suppose

$$Z = \begin{pmatrix} X & \alpha \\ \alpha^* & \beta \end{pmatrix} \in K$$

is N-block diagonalizable. Hence there exists a t and tuples $E^1, \ldots, E^t$ in K of size at most N and a unitary U such that $Z = U^*EU$, where

(4.1) $$E = \oplus_{\ell=1}^{t} E^\ell \in K.$$

Letting $C_1, \ldots, C_t$ denote the block entries of the first column of U with respect to the direct sum decomposition of E, it follows that

$$X = \sum_\ell C_\ell^* E^\ell C_\ell$$

and of course $\sum_\ell C_\ell^* C_\ell = I$. By Lemma 4.5, since X is matrix extreme and the size of E^ℓ is at most N, for each ℓ either $C_\ell = 0$ or E^ℓ is unitarily equivalent to X; without loss of

generality we may assume that either $E^\ell = X$ or $C_\ell = 0$. Let $\mathcal{J}$ denote the set of indices ℓ for which $E^\ell = X$. In particular, without loss of generality,

$$(4.2) \qquad\qquad X = \sum_\ell C_\ell^* X C_\ell.$$

From Proposition 4.6, each C_ℓ is a scalar multiple of the identity.

To see that $\alpha = 0$, write U as a block $t \times 2$ matrix whose entries are compatible with Z and the decomposition of E in (4.1). In particular, $U_{\ell,1} = C_\ell$ is a multiple of the identity. Observe that

$$\alpha_k = \sum_\ell U_{\ell,1}^* X U_{\ell,2} = X \sum U_{\ell,1}^* U_{\ell,2} = 0,$$

and thus $\alpha = 0$. Hence X is in the block-Arveson boundary of K. ∎

Lemma 4.10. *The matrix extreme points of a matrix convex set K contain the irreducible points in its block-Arveson boundary.*

Proof. Suppose $X \in K(n)$ is both irreducible and in the block-Arveson boundary of K. To prove X is a matrix extreme point, suppose

$$X = \sum_{j=1}^t C_j^* E^j C_j$$

where each C_j is nonzero, $\sum_{j=1}^t C_j^* C_j = I$ and $E^j \in K(n_j)$ for some $n_j \le n$. In this case, let

$$C = \begin{pmatrix} C_1 \\ \vdots \\ C_t \end{pmatrix} \qquad \text{and} \qquad E = E^1 \oplus \cdots \oplus E^t$$

and observe that C is an isometry and $X = C^* E C$. Since X is in the block-Arveson boundary of K, it follows that $CX = EC$. It follows that $C_\ell X_k = E_k^\ell C_\ell$ for each ℓ and k. With ℓ fixed, an application of Lemma 3.14 implies E^ℓ is unitarily equivalent to $X \oplus Z^\ell$ for some $Z^\ell \in K$. On the other hand, the size of E^ℓ is no larger than the size of X and hence $Z^\ell = 0$. Thus E^ℓ is unitarily equivalent to X. An application of Lemma 4.5 completes the proof. ∎

5. Proof of Theorem 1.2

The converse part of Theorem 1.2 appears as [HKM+, Theorem 4.6]. For the reader's convenience we provide the short proof here. Suppose $X \in (\mathrm{co}^{\mathrm{mat}}\{\Omega\})^\circ$. In particular, $L_\Omega(X) \succeq 0$ and hence $X \in \mathcal{D}_\Omega$. Conversely, suppose $X \in \mathcal{D}_\Omega$. Let $Y \in \mathrm{co}^{\mathrm{mat}}(\{\Omega\})$ be given. By (3.1), $Y = V^*(I_\mu \otimes \Omega)V$. Hence,

$$(5.1) \qquad \begin{aligned} L_X(Y) &= I - \sum_{j=1}^g X_j \otimes Y_j = (I \otimes V)^* \left(I - \sum_{j=1}^g X_j \otimes [I_\mu \otimes \Omega_j] \right)(I \otimes V) \\ &\stackrel{u}{\sim} (I \otimes V)^*(I_\mu \otimes L_X(\Omega))(I \otimes V). \end{aligned}$$

Since $L_X(\Omega)$ is unitarily equivalent to $L_\Omega(X)$ and $X \in \mathcal{D}_\Omega$, it follows that $L_X(Y) \succeq 0$ and therefore $X \in (\mathrm{co}^{\mathrm{mat}}\{\Omega\})^\circ$ and the proof of the converse part of Theorem 1.2 is complete.

Suppose $K^\circ = \mathcal{D}_\Omega$ for some d and g-tuple $\Omega \in \mathbb{S}_d^g$ and (without loss of generality) Ω is a minimal defining tuple for $\mathcal{D}_\Omega$ and write $\Omega = \oplus_{j=1}^N \Omega^j$ where the Ω^j are irreducible and mutually not unitarily equivalent. By the first part of the proof, $K^\circ = (\mathrm{co}^{\mathrm{mat}}\{\Omega\})^\circ$ and by the bipolar theorem [EW97] (see also [HKM+, §4.2]), $K = \mathrm{co}^{\mathrm{mat}}(\{\Omega\})$. (Here we have used $0 \in K$) Evidently $\Omega \in K$ and to complete the proof it suffices to show Ω is an Arveson boundary point for K. To prove this statement, suppose $\alpha \in (\mathbb{C}^d)^g$, $\beta \in \mathbb{R}^g$ and

$$(5.2) \qquad Y = \begin{pmatrix} \Omega & \alpha \\ \alpha^* & \beta \end{pmatrix} \in K(d+1)$$

Since $Y \in \mathrm{co}^{\mathrm{mat}}(\{\Omega\})$, by equation (3.1)

$$(5.3) \qquad Y = V^*(I_m \otimes \Omega)V$$

for some m and isometry V. Equation (5.2) implies $\mathcal{D}_Y \subseteq \mathcal{D}_\Omega$. On the other hand, Equation (5.3) implies $\mathcal{D}_Y \supseteq \mathcal{D}_\Omega$. Hence $\mathcal{D}_Y = \mathcal{D}_\Omega$. Since also Ω is minimal defining, the Gleichstellensatz [HKM13, Corollary 3.18 or Theorem 3.12] (see also [Zal17]) applies and there is a unitary U such that

$$\begin{pmatrix} \Omega & \alpha \\ \alpha^* & \beta \end{pmatrix} = U^* \begin{pmatrix} \Omega & 0 \\ 0 & \gamma \end{pmatrix} U$$

for some γ. In particular, for each $1 \leq j \leq g$,

$$\begin{pmatrix} \Omega_j & \alpha_j \\ \alpha_j^* & \beta_j \end{pmatrix} = U^* \begin{pmatrix} \Omega_j & 0 \\ 0 & \gamma_j \end{pmatrix} U$$

By the eigenvalue interlacing result, Lemma 3.12, it follows that $\alpha_j = 0$ (and $\gamma_j = \beta_j$). Hence, via an application of Lemma 3.5, Ω is in the Arveson boundary of K. ∎

6. Free Simplices and Polar Duals of Free Spectrahedra

In this section we give a surprising use of extreme points for matrix convex sets. Namely, we show that the polar dual of a free spectrahedron $\mathcal{D}_A$ can only be a free spectrahedron if $\mathcal{D}_A(1)$ is a polytope (Corollary 6.3). If $\mathcal{D}_A(1)$ is a simplex, we show that $\mathcal{D}_A^\circ$ is a free spectrahedron (cf. Theorem 6.5).

6.1. The polar dual of a free spectrahedron is seldom a free spectrahedron.
In this subsection we use the theory of extreme points for matrix convex sets to show that if the polar dual of a free spectrahedron $\mathcal{D}_A$ is a free spectrahedron then $\mathcal{D}_A(1)$ is a polytope.

Proposition 6.1. *Let $K = \mathcal{D}_A$ be a free spectrahedron. The Euclidean extreme points of $\mathcal{D}_A(1)$ are Arveson boundary points of $\mathcal{D}_A$.*

Proof. Fix a Euclidean extreme point $x \in \mathcal{D}_A(1)$. In this case $L_A(x) = I - \sum A_j x_j$ has maximal kernel by Corollary 2.3. Suppose $a \in \mathbb{C}^g$, $b \in \mathbb{R}^g$ and

$$Y = \begin{pmatrix} x & a \\ a^* & b \end{pmatrix} \in \mathcal{D}_A(2).$$

Using $L(Y) \succeq 0$, it follows that $\ker(\Lambda_A(a)) \supseteq \ker(L_A(x))$. Thus, by Theorem 2.2, $a = 0$. By Lemma 3.5, x is an Arveson boundary point of $\mathcal{D}_A$. ∎

Remark 6.2. We point out that Proposition 6.1 does not extend to general matrix convex sets. Indeed, the polar dual K of a free spectrahedron $\mathcal{D}_A$ has only finitely many (non-equivalent) Arveson boundary points in each $K(m)$ by Theorem 1.2. However, it is easy to construct examples where $K(1)$ has infinitely many Euclidean extreme points.

Corollary 6.3. *If the polar dual of $K = \mathcal{D}_A$ is again a free spectrahedron, then $\mathcal{D}_A(1)$ is a polyhedron. In particular, if $\mathcal{D}_A(1)$ is a ball, then the polar of $\mathcal{D}_A$ is not a free spectrahedron.*

Proof. Without loss of generality, L_A is minimal. If $K^\circ = \mathcal{D}_B$ is again a free spectrahedron (with L_B minimal), then K has finitely many irreducible Arveson boundary points by Theorem 1.2. In particular, by Proposition 6.1, $K(1)$ has finitely many boundary points and is thus a polyhedron. For the final statement of the corollary, use that $\mathcal{D}_A^\circ(1) = \mathcal{D}_A(1)^\circ$ by [HKM+, Proposition 4.3] since $\mathcal{D}_A$ is matrix convex. ∎

Remark 6.4. If $\mathcal{C}$ is the free cube, then its polar dual is not a free spectrahedron [HKM13]. Indeed, its Arveson boundary points are exactly tuples $J = (J_1, \ldots, J_g)$ of symmetries, i.e., $J_j^* = J_j$ and $J_j^2 = I$. If $\mathcal{C}^\circ$ were a free spectrahedron, then $\mathcal{C}$ would contain only finitely many inequivalent irreducible points in its Arveson boundary. But, say for the case $n = 2$ (square), each tuple

$$\left(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} s & t \\ t & -s \end{pmatrix} \right)$$

with $|s| \neq 1$, $t > 0$ and $s^2 + t^2 = 1$ gives such points (at level two).

We next turn our attention to free simplices, where polar duals are again free simplices and thus free spectrahedra.

6.2. Free simplices.
The main result of this subsection is Theorem 6.5. It characterizes the absolute extreme points of a free simplex $\mathcal{D}$ (i.e., a matrix convex set $\mathcal{D} \subseteq \mathbb{S}^g$ whose scalar points $\mathcal{D}(1) \subseteq \mathbb{R}^g$ form a simplex). These are exactly Euclidean extreme points of $\mathcal{D}(1)$.

A free spectrahedron $\mathcal{D} \subseteq \mathbb{S}^g$ is a **free simplex** if it is bounded and there exists a diagonal tuple $A \in \mathbb{S}_{g+1}^g$ such that A is a minimal defining tuple for $\mathcal{D}$. In particular, $\mathcal{D} = \mathcal{D}_A$.

Theorem 6.5. *If $\mathcal{D}_A$ be a free simplex, then $\partial^{\mathrm{abs}}\mathcal{D}_A = \partial^{\mathrm{abs}}(\mathcal{D}_A)(1) = \partial^{\mathrm{Euc}}\mathcal{D}_A(1)$. Furthermore $\mathcal{D}_A = \mathrm{co}^{\mathrm{mat}}(\partial^{\mathrm{abs}}\mathcal{D}_A)$. Thus, a point is in the Arveson boundary of $\mathcal{D}_A$ if and only if it is, up to unitary equivalence, a direct sum of points from $\partial^{\mathrm{Euc}}\mathcal{D}_A(1)$. In particular, Arveson boundary points are commuting tuples.*

The proof will use the notation S^+ to denote the positive semidefinite elements of a subset S of a matrix algebra.

Proof. By boundedness, the set $\{I, A_1, \ldots, A_g\}$ is a linearly independent subset of the diagonal matrices in $\mathbb{S}_{g+1}$. Hence its span is the commutative C*-algebra $\mathscr{D}$ of diagonal matrices in $M_{g+1}(\mathbb{C})$. In particular, if $Z \in M_n(\mathscr{D})^+ = (M_n \otimes \mathscr{D})^+$ then Z is in fact in $\mathscr{D}^+ \otimes M_n^+$. If $X \in \mathcal{D}_A(n)$, then $L_A(X) \succeq 0$ and therefore $Z = L_A(X) \in \mathscr{D}^+ \otimes M_n^+$. It follows that there exists a positive integer N, $n \times n$ rank one matrices $P_j \in M_n^+$ and $Q_j \in \mathscr{D}^+$ for $1 \le j \le N$ such that $Z = \sum Q_j \otimes P_j$. For each j there is a tuple $x_j = (x_{j,0}, \ldots, x_{j,g}) \in \mathbb{R}^{g+1}$ with

$$Q_j = x_{j,0} I + \sum_{k=1}^{g} x_{j,k} A_k \succeq 0.$$

If $x_{j,0} \le 0$, then $\sum_{k=1}^{g} x_{j,k} A_k \succeq 0$, and the domain $\mathcal{D}_A(1)$ is unbounded. Hence $x_0 > 0$ and, by replacing P_j by $\frac{1}{x_{j,0}} P_j$, we may assume $x_{j,0} = 1$. Letting $x^j = (x_{j,1}, \ldots, x_{j,g}) \in \mathcal{D}_A(1)$, we thus have

$$Z = \sum_j L_A(x^j) \otimes P_j = I \otimes \sum_j P_j + \sum_{k=1}^{g} A_k \otimes \sum_j x_{j,k} P_j.$$

Since $Z = L_A(X) = I \otimes I + \sum_k A_x \otimes X_k$, the linear independence of $\{I, A_1, \ldots, A_g\}$ implies

$$\sum_{j=1}^{N} P_j = I, \qquad \sum_{j=1}^{N} x_{jk} P_j = X_k, \ k = 1, \ldots, g.$$

Let $P_j = u_j u_j^*$ for $u_j \in \mathbb{R}^n$, $V = \text{col}(u_1^*, \ldots, u_N^*)$, and $\Xi_k = x_{1k} \oplus \cdots \oplus x_{Nk}$. Then V is an isometry, and

$$X_k = V^* \Xi_k V.$$

Furthermore, the tuple $\Xi = (\Xi_1, \ldots, \Xi_g) \in \mathcal{D}_A$ since $\Xi = x^1 \oplus \cdots \oplus x^N$ and each $x^j \in \mathcal{D}_A(1)$. We conclude $\mathcal{D}_A$ is the matrix convex hull of $\partial^{\text{Euc}} \mathcal{D}_A(1)$. The rest of the theorem now follows easily. ∎

Corollary 6.6. *The matrix convex hull K of $g+1$ affine independent points in $\mathbb{R}^g$ is a free simplex if and only if 0 is in the interior of $K(1)$.*

Let $\{e_1, \ldots, e_{g+1}\}$ denote the standard orthonormal basis in $\mathbb{C}^{g+1}$. Let $\mathcal{N} \in \mathbb{S}_{g+1}^g$ denote the g-tuple with $\mathcal{N}_j = -e_j e_j^* + \frac{1}{g+1} e_{g+1} e_{g+1}^*$ for $1 \le j \le g$. Thus $X \in \mathcal{D}_\mathcal{N}$ if and only if $X_j \ge -I$ for $1 \le j \le g$ and $\sum X_j \le (g+1)I$. We call $\mathcal{D}_\mathcal{N}$ the **Naimark spectrahedron**. Because the affine linear mapping $\mathcal{T} : \mathbb{S}^g \to \mathbb{S}^{g+1}$ defined by $X_j \mapsto \frac{1}{g}(X_j + I)$ for $1 \le j \le g$ and $X_{g+1} \mapsto \frac{g+1}{g} X_j$, implements an affine linear bijection between $\mathcal{D}_\mathcal{N}$ and the set

$$\mathcal{S} = \{Y \in \mathbb{S}^{g+1} : Y_j \succeq 0, \ I = \sum Y_j\}.$$

The set $\mathcal{S}$ is not a spectrahedron (and hence not a free simplex), since it doesn't contain 0, but it is the translation of a free simplex.

Proposition 6.7. *A spectrahedron $\mathcal{D}_A \subseteq \mathbb{S}^g$ is a free simplex if and only if it is affine linearly equivalent to the Naimark spectrahedron.*

Proof. To prove the only if direction, it suffices to show if $\mathcal{D}_A$ is a free simplex, then it is affine linearly equivalent to

$$(6.1) \qquad \mathfrak{S} = \{Y \in \mathbb{S}^g : Y_j \succeq 0, I \succeq \sum Y_j\}.$$

Let $\mathbf{A}$ denote the $(g+1) \times g$ matrix whose j-th column is the diagonal of A_j. Since $\mathcal{D}_A$ is bounded, the tuple A is linearly independent. Thus, without loss of generality, the matrix $\mathbf{S} = (\mathbf{A}_{k,j})_{j,k=1}^g$, whose j-th column of S are the first g entries of the diagonal of A_j, is invertible. Let $\lambda = \mathbf{S}^{-1}\mathbf{1}$, where $\mathbf{1} \in \mathbb{R}^g$ is the vector with each entry equal to 1. Define $\mathcal{T} : \mathbb{S}^g \to \mathbb{S}^g$ by

$$Z = \mathcal{T}(X) = \mathbf{S}(\lambda - X) = \mathbf{1} + \mathbf{S}X.$$

Thus $\mathcal{T}$ is an affine linear map and $Z_j = I + \sum_{s=1}^g \mathbf{A}_{j,s} X_s$. Since $\mathcal{D}_A$ is bounded and non-empty, the same is true of $\mathcal{T}(\mathcal{D}_A)$. Further, $I + \sum_{s=1}^g \mathbf{A}_{j,s} X_s \succeq 0$ if and only if $Z_j \succeq 0$. Moreover, since

$$I \succeq \sum_s \mathbf{A}_{g+1,s} X_s = \sum_t \left[\sum_s \mathbf{A}_{g+1,s}(\mathbf{S}^{-1})_{s,t}\right](Z_t - I),$$

$I + \sum_s \mathbf{A}_{g+1,s} X_s \succeq 0$ if and only if $I + \sum_t \beta_t I \succeq \sum \beta_t Z_t$, where $\beta_t = \sum_s \mathbf{A}_{g+1,s}(\mathbf{S}^{-1})_{s,t}$. Hence $X \in \mathcal{D}_A$ if and only if

$$Z_j \succeq 0, \ I + \sum \beta_t \succeq \sum \beta_t Z_t.$$

Since the set of such Z, namely $\mathcal{T}(\mathcal{D}_A)$ is bounded, $\beta_t > 0$ for each t. Replacing Z_t by $Y_t = \frac{\beta_t}{1+\sum \beta_t} Z_t$ we have mapped $\mathcal{D}_A$ to $\mathfrak{S}$ via a bijective affine linear transformation.

For the converse, suppose A is a minimal defining tuple for $\mathcal{D}_A$ and $\mathcal{D}_A$ is affine linearly equivalent to $\mathcal{D}_{\mathscr{N}}$ via an affine linear map $\mathcal{T}$. Thus, there exists scalars $(b_{j,k})$ and c_j for $1 \le j, k \le g$ such that $X \in \mathcal{D}_{\mathscr{N}}$ if and only if the tuple $\mathcal{T}(X)$ defined by

$$\mathcal{T}(X)_j = \sum_{k=1}^g b_{j,k} X_k + c_j I$$

is in $\mathcal{D}_A$. Thus, $X \in \mathcal{D}_{\mathscr{N}}$ if and only if

$$I + \sum_{j=1}^g A_j \otimes \left[\sum_k b_{j,k} X_K + c_j I\right] \succeq 0.$$

Rearranging,

$$[I + \sum c_j A_j] + \sum_k \sum_j (A_j b_{j,k}) \otimes X_k \succeq 0.$$

Choosing $X = 0$, it follows that $I + \sum c_j A_j \succ 0$. Let P denote the positive square root of this operator and let $B_k = P^{-1} \sum_j (A_j b_{j,k}) P^{-1}$. With this notation, $X \in \mathcal{D}_{\mathcal{N}}$ if and only if

$$I + \sum_{k=1}^{n} B_k \otimes X_k \succeq 0.$$

Thus $\mathcal{D}_{\mathcal{N}} = \mathcal{D}_B$. Since A is a minimal defining tuple for $\mathcal{D}_A$, the tuple B is minimal defining for $\mathcal{D}_B$. It follows from the Gleichstellensatz ([HKM13, Corollary 3.18 or Theorem 3.12]; see also [Zal17]), that $\mathcal{N}$ and B are unitarily equivalent and in particular B (and hence A) has size $g+1$ and B is a tuple of commuting self adjoint matrices. Moreover, for some scalars α_k,

$$I - P^{-2} = \sum \alpha_k B_k.$$

Hence P^{-2} commutes with each B_k and since P is positive definite, so does P. Consequently the matrices $B_k' = \sum_j b_{j,k} A_j$ commute and since the matrix $(b_{j,k})$ is invertible, A is a tuple of commuting matrices of size $g + 1$ and the proof is complete. ∎

Corollary 6.8. *The polar dual of a free simplex is a free simplex.*

Proof. Assume $\mathcal{D}_A$ is a free simplex and let $\omega = \partial^{\mathrm{Euc}} \mathcal{D}_A(1) \subseteq \mathbb{R}^g$. Then ω has $g+1$ elements by Proposition 6.7. Build the corresponding diagonal matrices $\Omega_j \in \mathbb{S}_{g+1}$, $j = 1, \ldots, g$. Then by Theorem 6.5, $\mathcal{D}_A = \mathrm{co}^{\mathrm{mat}}(\{\Omega\})$. Thus by Theorem 1.2, $\mathcal{D}_A^\circ = \mathcal{D}_\Omega$ is a free simplex. ∎

In [FNT+] Fritz, Netzer and Thom use extreme points to investigate when an abstract operator system has a finite-dimensional concrete realization. They show that the maximal operator system above a convex set $C \subseteq \mathbb{R}^g$ is a free spectrahedron if and only if C is a polyhedron containing 0 in its interior [FNT+, Theorem 3.2]. Similarly, among such $C \subseteq \mathbb{R}^g$, the minimal operator system above C is a free spectrahedron if and only if C is a simplex [FNT+, Theorem 4.7].

7. Applications

In this section we give further applications of the theory of matrix convex sets. Subsection 7.1 characterizes extreme points of the free cube. In Subsection 7.2 the theory of extreme points is applied to the study of free spectrahedra $\mathcal{D}_A$ such that $\mathcal{D}_A(1)$ is the unit disk $\{(x,y) \in \mathbb{R}^2 : x^2 + y^2 \leq 1\}$. In Subsection 7.3 extreme points are used to analyze the matrix convex hull of the TV screen $\{(X,Y) : I - X^2 - Y^4 \succeq 0\} \subseteq \mathbb{S}^2$.

7.1. **Free cube.** As noted in Section 6.1, the Arveson boundary points of the free cube $\mathcal{C} = \{X \in \mathbb{S}^g : \|X_i\| \leq 1 \text{ for } 1 \leq i \leq g\}$ are exactly tuples $J = (J_1, \ldots, J_g)$ of symmetries. In this section we show each Euclidean extreme point of $\mathcal{C}$ is an Arveson boundary point.

Proposition 7.1. *Let $\mathcal{C} \subseteq \mathbb{S}^g$ be the free cube. Then $\partial^{\mathrm{Euc}} \mathcal{C} = \partial^{\mathrm{arv}} \mathcal{C}$.*

Proof. Letting $\{e_1, \ldots, e_g\}$ denote the standard basis of $\mathbb{C}^g$, and $A_j = (e_j e_j^*) \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ for $1 \leq j \leq g$, we have $\mathcal{C} = \mathcal{D}_A$. We shall use the Arveson-like characterization (Corollary 2.3) of Euclidean extreme points of $\mathcal{D}_A$.

Let $X \in \partial^{\mathrm{Euc}}\mathcal{D}_A(n)$. That is, $X \in \mathcal{D}_A(n)$ is such that $\ker L_A(X) \subseteq \ker \Lambda_A(Y)$ for $Y \in \mathbb{S}_n^g$ implies $Y = 0$. Assume that $X_j^2 \neq 1$ for some j. Without loss of generality, $j = 1$. Let $0 \neq u \in \mathbb{C}^n$ be any vector orthogonal to $\ker(I - X_1^2)$ and form the tuple $Y \in \mathbb{S}_n^g$ by $Y_1 = uu^*$ and $Y_k = 0$ for $k \geq 2$. Then $\ker L_A(X) \subseteq \ker \Lambda_A(Y)$ and $Y \neq 0$, violating $X \in \partial^{\mathrm{Euc}}\mathcal{D}_A$. This contradiction shows $X_j^2 = I$ for all j, i.e., $\partial^{\mathrm{Euc}}\mathcal{C} \subseteq \partial^{\mathrm{arv}}\mathcal{C}$. The converse inclusion is obvious. $\blacksquare$

7.2. Disks.

In this subsection we study the extreme points of two different free spectrahedra whose scalar points describe the unit disk.

7.2.1. *Arveson boundary of the Wild Disk.*

Consider the pencil

$$L_A(x) = \begin{pmatrix} 1 & x_1 & x_2 \\ x_1 & 1 & 0 \\ x_2 & 0 & 1 \end{pmatrix}$$

The domain $\mathcal{D}_A$ is the **wild disk**. Note that $X \in \mathcal{D}_A$ if and only if $p(X) = I - X_1^2 - X_2^2 \succeq 0$. In anticipation of the forthcoming flood of subscripts we change the notation (X_1, X_2) to (X, Y) here in Subsection 7.2.1 and in Section 7.3.

We now give an estimate on the size of the kernel of $L_A(X, Y)$ for (X, Y) an Arveson boundary point. Suppose (X, Y) has size $3n$ and $L_A(X, Y) \succeq 0$. Let $\mathcal{K}$ denote the kernel of $p(X, Y)$. A straightforward computation shows $k \in \mathcal{K}$ if and only if

$$(7.1) \qquad \qquad \begin{pmatrix} k & -Xk & -Yk \end{pmatrix}^* \in \ker(L_A(X)).$$

Write $\mathbb{C}^n = \mathcal{K} \oplus \mathcal{K}^\perp$. Suppose $\gamma = (\alpha, \beta) \in M_{n,2}(\mathbb{C}^2) = \mathbb{C}^{n \times 2}$ and

$$\ker(L_A(X)) \subseteq \ker(\Lambda_A(\gamma)^*).$$

It is readily verified that this inclusion is equivalent to

$$(\alpha^* X + \beta^* Y)k = 0$$
$$(7.2) \qquad \qquad\qquad\qquad \alpha^* k = 0$$
$$\beta^* k = 0$$

for all $k \in \mathcal{K}$. The last two relations imply that $\alpha, \beta \in \mathcal{K}^\perp$. Let P denote the projection onto $\mathcal{K}^\perp$ and $Q = I - P$ the projection onto $\mathcal{K}$. Further, let $X_{12} = QXP$ and similarly for Y_{12}.

Lemma 7.2. *There is no nontrivial solution $\gamma = (\alpha, \beta)$ to the system (7.2) (equivalently (X, Y) is in the Arveson boundary of $\mathcal{D}_A$) if and only if both X_{12} and Y_{12} are one-to-one and $\mathrm{rg}(X_{12}) \cap \mathrm{rg}(Y_{12}) = (0)$.*

Proof. First suppose $0 \neq \alpha \in \mathcal{K}^{\perp}$ and $X_{12}\alpha = 0$. In this case the pair $\gamma = (0 \oplus \alpha, 0)$ is a non-trivial solution to the system (7.2). Thus, both X_{12} (and by symmetry) Y_{12} are one-to-one.

Next suppose there exists $u, v \in \mathcal{K}^{\perp}$ such that $X_{12}u = Y_{12}v \neq 0$. In this case $\gamma = (0 \oplus u, -0 \oplus v)$ is a nontrivial solution to the system in (7.2). ∎

Lemma 7.3. *If (X, Y) has size $3N$ and is in the Arveson boundary, then the kernel of $p(X, Y)$ has dimension at least $2N$. Thus the dimension of $\mathcal{K}$ is at least two-thirds the size of (X, Y).*

Proof. Let m denote the dimension of $\mathcal{K}$. From Lemma 7.2, it follows that the dimensions of $\mathrm{rg}(X_{12})$ and of $\mathrm{rg}(Y_{12})$ are both $3N - m$ as subspaces of a space of dimension m. The intersection of these ranges is nonempty if $6N - 2m = 2(3N - m) > m$. Hence, if X is in the Arveson boundary, then $6N \leq 3m$. ∎

Proposition 7.4. *If (X, Y) has size n and the dimension of the kernel $\mathcal{K}$ of $p(X, Y)$ is $n - 1$, then either (X, Y) is in the Arveson boundary or (X, Y) dilates to a pair $(\tilde{X}, \tilde{Y})$ of size $n + 1$ which lies in the vanishing boundary of $\mathcal{D}_A$; i.e., $p(\tilde{X}, \tilde{Y}) = 0$.*

Proof. Suppose (X, Y) is not in the Arveson boundary. In this case the analysis above applies and since $\alpha, \beta \in \mathcal{K}^{\perp}$, they are multiples of a single unit vector u. With a slight change of notation, write $\alpha = \alpha u$ and $\beta = \beta u$. Express X (and similarly Y) with respect to the decomposition $\mathcal{K} \oplus \mathcal{K}^{\perp}$ as

$$X = \begin{pmatrix} X_{11} & X_{12} \\ X_{12}^* & x_{22} \end{pmatrix}.$$

The vector $\begin{pmatrix} X_{12}^* & x_{22} \end{pmatrix}^*$ is Xu and $X_{12} = QXu$, where, as before, Q is the projection onto K. The relation $QX\alpha + QY\beta = 0$ implies that the vectors X_{12} and Y_{12} are co-linear. Accordingly, write $X_{12} = x_{12}e$ and likewise $Y_{12} = y_{12}e$ for some unit vector e. Let t be a real parameter, and a, b numbers all to be chosen soon. Consider,

$$\tilde{X} = \begin{pmatrix} X_{11} & x_{12}e & 0 \\ x_{12}e^* & x_{22} & t\alpha \\ 0 & t\alpha & a \end{pmatrix}$$

and similarly for $\tilde{Y}$. We have,

$$I - \tilde{X}^2 - \tilde{Y}^2 = \begin{pmatrix} 0 & -(x_{12}(X_{11} + x_{22}) + y_{12}(Y_{11} + y_{22}))e & t(x_{12}\alpha + y_{12}\beta)e \\ * & 1 - [x_{12}^2 + x_{22}^2 + y_{12}^2 + y_{22}^2 + t^2(\alpha^2 + \beta^2)] & t[(x_{22} + a)\alpha + (y_{22} + b)\beta] \\ * & * & 1 - t^2(\alpha^2 + \beta^2) - a^2 - b^2 \end{pmatrix}.$$

The $(1, 2)$ entry is 0 since $(X, Y) \in \mathcal{D}_A$. Likewise the $(1, 3)$ entry is 0 by the relations in Equation (7.2). The parameter t is determined, up to sign, by setting the $(2, 2)$ entry equal to zero.

Let Γ denote the vector $\begin{pmatrix} \alpha & \beta \end{pmatrix}^*$ and Δ the vector $\begin{pmatrix} a & b \end{pmatrix}^*$. Thus,

$$t^2\|\Gamma\|^2 = 1 - [x_{12}^2 + x_{22}^2 + y_{12}^2 + y_{22}^2] \geq 0.$$

We hope to find Δ so that

(7.3)
$$t^2\|\Gamma\|^2 = 1 - \|\Delta\|^2$$
$$\langle \Delta, \Gamma \rangle = \langle \Sigma, \Gamma \rangle,$$

where $\Sigma = \begin{pmatrix} x_{22} & y_{22} \end{pmatrix}^*$. Note that the first equation of (7.3) determines the norm of Δ. The claim is that these equations have a solution if $\|\Delta\| \geq \|\Sigma\|$. Now,

$$\|\Delta\|^2 = 1 - t^2\|\Gamma\|^2 = [x_{12}^2 + x_{22}^2 + y_{12}^2 + y_{22}^2] \geq \|\Sigma\|^2. \qquad \blacksquare$$

We do not know if either the matrix convex hull or the closed matrix convex hull of the Arveson boundary of $\mathcal{D}_A$ is all of $\mathcal{D}_A$. Since one can construct $n \times n$ pairs (X_1, X_2) in the Arveson boundary of $\mathcal{D}_A$ such that $I - X_1^2 - X_2^2 \neq 0$, the matrix convex hull of the vanishing boundary of $\mathcal{D}_A$ is not all of $\mathcal{D}_A$. We do not know if the same is true of the closed matrix convex hull of the vanishing boundary.

7.2.2. *Arveson boundary of the Spin Disk.* Consider the pencil

$$L_A(x_1, x_2) = \begin{pmatrix} 1 + x_1 & x_2 \\ x_2 & 1 - x_1 \end{pmatrix}.$$

The free spectrahedron $\mathcal{D}_A$ is the **spin disk**. It is the $g = 2$ case of a **spin ball** [HKMS+, DDSS+].

Proposition 7.5. *A pair $(X_1, X_2) \in \mathbb{S}^2$ is in the Arveson boundary of $\mathcal{D}_A$ if and only if X_1 and X_2 commute and $p(X_1, X_2) = I - X_1^2 - X_2^2 = 0$. Furthermore,*

(7.4)
$$\mathrm{co}^{\mathrm{mat}}(\partial^{\mathrm{arv}}\mathcal{D}_A) = \mathcal{D}_A.$$

As an immediate consequence, the set of absolute extreme points of $\mathcal{D}_A$ equals the Euclidean extreme points of $\mathcal{D}_A(1)$.

Proof. Recall [HKMS+, Proposition 14.14]: a tuple $X \in \mathbb{S}^2$ is in $\mathcal{D}_A$ if and only if it dilates to a commuting pair T of self-adjoint matrices with joint spectrum in the unit disk $\mathbb{D} \subseteq \mathbb{R}^2$.

Suppose $X \in \partial^{\mathrm{arv}}\mathcal{D}_A$. Then by [HKMS+, Proposition 14.14], X_1 and X_2 commute. Without loss of generality, they are diagonal, say $X_j = \mathrm{diag}(c_{1j}, \ldots, c_{nj})$. Clearly, $c_{i1}^2 + c_{i2}^2 = 1$ for all i as otherwise the tuple X will obviously have a nontrivial dilation. In particular, $p(X_1, X_2) = 0$.

Conversely, assume X_1 and X_2 commute and $p(X_1, X_2) = 0$. Suppose $\hat{X} \in \mathcal{D}_A$ with

$$\hat{X}_j = \begin{pmatrix} X_j & \alpha_j \\ \alpha_j^* & \beta_j \end{pmatrix}$$

Since $\mathcal{D}_A$ is contained in the wild disk (see e.g. [HKM13, Example 3.1]), the tuple $\hat{X}$ is in the wild disk and thus $p(\hat{X}_1, \hat{X}_2) \succeq 0$. Compute

$$p(\hat{X}_1, \hat{X}_2) = I - \hat{X}_1^2 - \hat{X}_2^2 = \begin{pmatrix} I - X_1^2 - X_2^2 - \alpha_1\alpha_1^* - \alpha_2\alpha_2^* & * \\ * & * \end{pmatrix} = \begin{pmatrix} -\alpha_1\alpha_1^* - \alpha_2\alpha_2^* & * \\ * & * \end{pmatrix}.$$

By positive semidefiniteness, $\alpha_1 \alpha_1^* + \alpha_2 \alpha_2^* = 0$ and thus $\alpha_1 = \alpha_2 = 0$, i.e., $X \in \partial^{\mathrm{arv}} \mathcal{D}_A$.

Finally, to prove (7.4), let $X \in \mathcal{D}_A$ be arbitrary. By [HKMS+, Proposition 14.14], X dilates to a commuting pair $T \in \mathbb{S}^2$ with joint spectrum in $\mathbb{D}$. By diagonalizing we can thus reduce to $X \in \mathcal{D}_A(1)$. By employing usual convex combination, we can write $X = \sum_{j=1}^{2} \lambda_j Y^j$, where each $\lambda_j \geq 0$, $Y^j \in \mathbb{R}^2$ with $\sum \lambda_j = 1$ and $\|Y^j\| = 1$. Thus

$$X = V^*(Y^1 \oplus Y^2)V$$

for the isometry $V = \left(\sqrt{\lambda_1} \quad \sqrt{\lambda_2} \right)^*$. By the above, $Y^1 \oplus Y^2 \in \partial^{\mathrm{arv}} \mathcal{D}_A$, concluding the proof. ∎

Remark 7.6. One way to see that the wild disk and the spin disk are distinct is to observe that any non-commuting pair $(X, Y) \in \mathbb{S}^2$ satisfying $I - X^2 - Y^2 = 0$ is in the wild disk, but not necessarily in the spin disk. If it were in the spin disk, it would dilate to a commuting pair $(\tilde{X}, \tilde{Y})$ in the spin disk and hence in the wild disk. But (X, Y) is in the Arveson boundary of the wild disk and hence this dilation would simply contain (X, Y) as a direct summand and hence $(\tilde{X}, \tilde{Y})$ would then not commute.

7.3. **TV screen** $p = 1 - x^2 - y^4$. In this section we consider the extreme points of the matrix convex hull $\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$ of the free semialgebraic set $\mathcal{D}_p$ associated to $p = 1 - x^2 - y^4$, i.e., the TV screen,

$$\mathcal{D}_p = \{(X, Y) \in \mathbb{S}^2 : I - X^2 - Y^4 \succeq 0\}.$$

An important question is how to compute the matrix convex hull of a general free semialgebraic set. In the commutative case, a standard and well studied approach involves representing the convex hull of a semialgebraic set as a spectrahedrop; i.e., the projection of a spectrahedron living in higher dimensions. The set $\mathcal{D}_p(1) = \{(x, y) \in \mathbb{R}^2 : 1 - x^2 - y^4 \geq 0\}$ is of course convex. However already $\mathcal{D}_p(2)$ is not. Thus $\mathcal{D}_p$ is arguably the simplest non-convex free semialgebraic set. By using extreme point analysis on a natural free spectrahedrop approximation of $\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$, we will see that the spectrahedrop paradigm behaves poorly in the free setting.

A natural approximation [HKM16] to the matrix convex hull $\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$ of $\mathcal{D}_p$ is the projection $\mathcal{C}$ onto x, y-space of the matrix convex set

$$\widehat{\mathcal{D}_p} = \{(X, Y, W) \in \mathbb{S}^3 : I - X^2 - W^2 \succeq 0, \ \ W \succeq Y^2\}.$$

Clearly,

$$\mathcal{C} = \{(X, Y) \in \mathbb{S}^2 : \ \exists W \in \mathbb{S} \ \ I - X^2 - W^2 \succeq 0, \ \ W \succeq Y^2\}.$$

Lemma 7.7.

(1) $\mathcal{C}(1) = \mathcal{D}_p(1)$;
(2) $\mathcal{D}_p \subseteq \mathcal{C}$;
(3) $\mathcal{C}$ is matrix convex;
(4) $\mathcal{C}$ is a free spectrahedrop, i.e., a projection of a free spectrahedron.

Proof. These statements are straightforward to prove. The simplest LMI representation for $\widehat{\mathcal{D}_p}$ in (4) is given by

$$\Lambda = \begin{pmatrix} 1 & 0 & x \\ 0 & 1 & w \\ x & w & 1 \end{pmatrix} \oplus \begin{pmatrix} 1 & y \\ y & w \end{pmatrix},$$

i.e., $\mathcal{D}_\Lambda = \widehat{\mathcal{D}_p}$. This is seen by using Schur complements. It is easy to convert this LMI representation to a monic one [HKM16]. Let

$$L_1(x,y,w) = \begin{pmatrix} 1 & \gamma y \\ \gamma y & w + \alpha \end{pmatrix}, \quad L_2(x,y,w) = \begin{pmatrix} 1 & 0 & \gamma^2 x \\ 0 & 1 & w \\ \gamma^2 x & w & 1 - 2\alpha w \end{pmatrix}$$

where $\alpha > 0$ and $1 + \alpha^2 = \gamma^4$, and set $L = L_1 \oplus L_2$. While strictly speaking L is not monic, it contains 0 in its interior, so can be easily modified to become monic [HV07, Lemma 2.3]. ∎

It is tempting to guess that $\mathcal{C}$ actually is the matrix convex hull of $\mathcal{D}_p$, but alas

Proposition 7.8. $\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p) \subsetneq \mathcal{C}$.

A proof of this proposition appears in [HKM16] and is by brute force verification that the point in equation (7.9) below is in $\mathcal{C}$ but not $\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$. Here we shall give some conceptual justification for why $\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p) \neq \mathcal{C}$ based on our notions of extreme points. In the process we illustrate some features of the Arveson boundary.

7.3.1. *The vanishing boundary.* We define the **vanishing boundary** of $\mathcal{D}_p$ to be all $X \in \mathcal{D}_p$ making $p(X) = 0$. Let $\partial^{\mathrm{van}}\mathcal{D}_p$ denote the set of all vanishing boundary points.

Lemma 7.9. $\partial^{\mathrm{van}}\mathcal{D}_p \subseteq \partial^{\mathrm{arv}}\mathcal{D}_p$.

Proof. Assuming $p(X,Y) = 0$, suppose

$$Z = \begin{pmatrix} X & \alpha \\ \alpha^* & A \end{pmatrix}, \qquad W = \begin{pmatrix} Y & \beta \\ \beta^* & B \end{pmatrix}$$

and $p(Z,W) \succeq 0$. The $(1,1)$ entry of $p(Z,W)$ is

$$1 - X^2 - \alpha\alpha^* - (Y^2 + \beta\beta^*)^2 - \Gamma\Gamma^*$$

for some Γ. Using $p(X,Y) = 0$ and letting $Q = \beta\beta^*$, it follows that

$$QY^2 + Y^2Q + Q^2 \preceq 0.$$

Now apply the trace and note the trace of QY^2 is the same as the trace of YQY so is nonnegative. The conclusion is that the trace of Q^2 is zero and hence $Q = 0$ and $\beta = 0$. Thus $-\alpha\alpha^* - \Gamma\Gamma^* \succeq 0$, so $\alpha = 0$. ∎

7.3.2. *Some Arveson boundary points in $\mathcal{C}$.* Here we produce classes of interesting points in $\partial^{\mathrm{arv}}\mathcal{C}$. Consider the set of points (X, Y, W), denoted $\widehat{A}$, in $\widehat{\mathcal{D}}_p$ such that $I - X^2 - W^2 = 0$ and $W - Y^2$ is a rank one positive semidefinite matrix J. An association of $\widehat{A}$ to the Arveson boundary is given in the next proposition.

Proposition 7.10. *Suppose $(X, Y, W) \in \widehat{A}$ and $J = W - Y^2 \neq 0$ (of course, J is rank one and positive semidefinite).*

(1) *If $(X, Y) \notin \mathcal{D}_p$, then*
    (a) *the lift (X, Y, W) of (X, Y) to $\widehat{\mathcal{D}}_p$ is unique, i.e., if also $(X, Y, S) \in \widehat{\mathcal{D}}_p$ then $S = W$;*
    (b) *$(X, Y) \in \partial^{\mathrm{arv}}\mathcal{C}$ and $(X, Y, W) \in \partial^{\mathrm{arv}}\widehat{\mathcal{D}}_p$;*
    (c) *$(X, Y) \in \mathcal{C} \setminus \mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$.*
(2) *If $(X, Y) \in \mathcal{D}_p(n)$, then (X, Y, W) is a not a Euclidean extreme point of $\widehat{\mathcal{D}}_p(n)$ and (X, Y) is not a Euclidean extreme point of $\mathcal{C}$.*

If $J = 0$, then $W = Y^2$, so $(X, Y, Y^2) \in \partial^{\mathrm{arv}}\widehat{\mathcal{D}}_p$, $(X, Y) \in \partial^{\mathrm{arv}}\mathcal{C}$, and $(X, Y) \in \partial^{\mathrm{arv}}\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$.

7.3.3. *Proof of Proposition 7.10.* We begin the with several lemmas.

Lemma 7.11 (Paul Robinson private communication). *Suppose E and P are positive semi-definite matrices and $J \succeq 0$ is rank one. If*

$$(E + P)^2 \preceq (E + J)^2,$$

then $P = J$ or $JE = EJ = \lambda J$ for a scalar $\lambda \geq 0$.

An amusing case is when $P = 0$. Here $E \preceq E + J$, and the lemma says $E^2 \not\preceq (E + J)^2$ unless $JE = EJ = \lambda J$.

Proof. The square root function is operator monotone. Hence, $(E + P)^2 \preceq (E + J)^2$ implies $E + P \preceq E + J$ and thus $P \preceq J$. Since J is rank one, there is a $0 \leq t \leq 1$ so that $P = tJ$. Thus,

$$(E + tJ)^2 \preceq (E + J)^2$$

from which it follows that

$$0 \preceq (1 - t)(EJ + JE + (1 + t)J^2).$$

Since $0 \leq t \leq 1$, it now follows that if P is not equal to J (so $t < 1$) that

$$0 \preceq EJ + JE + 2J^2.$$

Using $J^2 = sJ$ for some $s > 0$, one finds

(7.5)
$$0 \preceq RR^* - \frac{1}{2s^2}(EJ^2E)$$

where R is the rank one matrix

(7.6)
$$R = (\sqrt{2} + \frac{1}{\sqrt{2s}}E)J.$$

If $EJ = 0$, then the conclusion holds with $\lambda = 0$. If $EJ \neq 0$, then (7.5) implies the range of R is equal to the range of EJ. However, combining this range equality with (7.6), gives the range of J equals the range of EJ. Thus EJ and J are both rank one with the same range and kernel. It follows that EJ is a multiple of J. Since E and J are both self-adjoint, E and J commute. Finally, E and J are, by hypothesis, positive semidefinite. Hence $EJ = \lambda J$ for some $\lambda > 0$. ∎

Lemma 7.12. *Suppose* $(X, Y, W) \in \widehat{A}$ *and let* $J = W - Y^2 \neq 0$. *Thus* J *is rank one and positive semidefinite. If* $(X, Y, S) \in \widehat{\mathcal{D}_p}$, *the either*

(A) $S = W$; *or*
(B) *there is a* $\lambda > 0$ *such that* $Y^2 J = \lambda J$.

Proof. Since $(X, Y, S) \in \widehat{\mathcal{D}_p}$, we have $I - X^2 \succeq S^2$ and there is a positive semidefinite matrix P such that $S = Y^2 + P$. On the other hand, $(X, Y, W) \in \widehat{A}$ gives $I - X^2 = W^2$ and $W = Y^2 + J$. Hence $W^2 \succeq S^2$. Equivalently,

$$(Y^2 + J)^2 \succeq (Y^2 + P)^2.$$

By Lemma 7.11, either $P = J$ or $JY^2 = Y^2 J = \lambda J$ for some $\lambda \geq 0$. ∎

We are now ready to prove Proposition 7.10 (1) which we restate as a lemma.

Lemma 7.13. *If* $(X, Y, W) \in \widehat{A}$, $(X, Y, S) \in \mathcal{C}$, *but* $(X, Y) \notin \mathcal{D}_p$, *then* $S = W$ *and* $(X, Y) \in \partial^{\mathrm{arv}} \mathcal{C} \setminus \mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$ *and* $(X, Y, W) \in \partial^{\mathrm{arv}} \widehat{\mathcal{D}_p}$.

Proof. From Lemma 7.12, there are two cases to consider. In case (B), $W^2 \succeq Y^4 + \sigma J$ for a $\sigma \geq 0$ and hence $I - X^2 - Y^4 \succeq I - X^2 - W^2 = 0$ so that $(X, Y) \in \mathcal{D}_p$. Thus, case (A) holds; i.e., $S = W$. In particular, $I - X^2 - S^2 = 0$.

Suppose the tuple

$$(7.7) \qquad \tilde{X} = \begin{pmatrix} X & \alpha \\ \alpha^* & * \end{pmatrix}, \quad \tilde{Y} = \begin{pmatrix} Y & \beta \\ \beta^* & Y_* \end{pmatrix}, \quad \tilde{S} = \begin{pmatrix} S & t \\ t^* & S_* \end{pmatrix}.$$

is in $\widehat{\mathcal{D}_p}$. Positivity of the upper left entry of $\tilde{S} - \tilde{Y}^2$ gives $S \succeq Y^2 + \beta\beta^*$ and positivity of the upper left entry of $I - \tilde{X}^2 - \tilde{S}^2$ gives

$$I - X^2 - S^2 \succeq \alpha\alpha^* + t^* t \succeq 0.$$

From what has already been proved, $S = W$ and $I - X^2 - S^2 = 0$. Hence $\alpha = t = 0$.

To show $\beta = 0$, observe the inequality $\tilde{S} \succeq \tilde{Y}^2$ implies

$$\begin{pmatrix} S & 0 \\ 0 & S_* \end{pmatrix} - \begin{pmatrix} Y^2 + \beta\beta^* & Y\beta + \beta Y_* \\ (Y\beta + \beta Y_*)^* & Y_*^2 + \beta^*\beta \end{pmatrix} \succeq 0.$$

Hence,

$$(7.8) \qquad \begin{pmatrix} J - \beta\beta^* & -(Y\beta + \beta Y_*) \\ -(Y\beta + \beta Y_*)^* & S_* - (Y_*^2 + \beta^*\beta) \end{pmatrix} \succeq 0.$$

Since the left top corner is positive and J is rank one, $\beta\beta^* = aJ$ for some $0 \leq a \leq 1$. If $a = 0$, then $\beta = 0$. Arguing by contradiction, suppose $a \neq 0$. The inequality of equation (7.8) implies there is a matrix C such that $Y\beta + \beta Y_* = JC$. Rearranging and multiplying on the right by β^* gives

$$Y\beta\beta^* = \beta\left(-Y_* + \frac{\beta^*}{a}C^*\right)\beta^*.$$

Since β is rank one ($\beta\beta^* = aJ$ and J is rank one), we conclude, $Y\beta\beta^* = b\beta\beta^*$ and thus $YJ = bJ$. It now follows that $W^2 = (Y^2 + J)^2 = Y^4 + 2ab^2J + J^2 \succeq 0$ and hence

$$I - X^2 - Y^4 \succeq I - X^2 - W^4 \succeq 0.$$

Consequently, $(X, Y) \in \mathcal{D}_P$, a contradiction.

Summarizing, if $\tilde{X}$, $\tilde{Y}$ and $\tilde{S}$ are as in equation (7.7) and $(\tilde{X}, \tilde{Y}, \tilde{S}) \in \widehat{\mathcal{D}_p}$, then $S = W$ and $\alpha = \beta = t = 0$. It is immediate that $(X, Y, W) \in \partial^{\mathrm{arv}}\widehat{\mathcal{D}_p}$. To prove $(X, Y) \in \partial^{\mathrm{arv}}\mathcal{C}$, suppose $\tilde{X}$ and $\tilde{Y}$ are as in equation (7.7) and $(\tilde{X}, \tilde{Y}) \in \mathcal{C}$. Thus, there is a $\tilde{S}$ such that $(\tilde{X}, \tilde{Y}, \tilde{S}) \in \widehat{\mathcal{D}_p}$. Express $\tilde{S}$ as in equation (7.7) too. It follows that $\alpha = \beta = 0$. Hence $(X, Y) \in \partial^{\mathrm{arv}}\mathcal{C}$. Finally, arguing by contradiction, suppose $(X, Y) \in \mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$. In this case, $(X, Y) \in \partial^{\mathrm{arv}}\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p)$ since $\mathrm{co}^{\mathrm{mat}}(\mathcal{D}_p) \subseteq \mathcal{C}$ and $(X, Y) \in \partial^{\mathrm{arv}}\mathcal{C}$. An application of Lemma 3.7 gives the contradiction $(X, Y) \in \mathcal{D}_p$. ∎

Proof of the remainder of Proposition 7.10. To prove item (2), suppose $(X, Y) \in \mathcal{D}_p$ and $(X, Y, W) \in \widehat{A}$. In particular, $I - X^2 - Y^4 \succeq 0$ and both $I - X^2 - W^2 = 0$ and $W - Y^2 = J$ is rank one positive semidefinite. Combining the first two of these equations gives $W^2 \succeq Y^4$. Using the third,

$$(Y^2 + J)^2 \succeq (Y^2)^2.$$

From Lemma 7.11, $Y^2J = \lambda J$. In particular Y^2 commutes with J (and so Y commutes with $J^{1/2}$). Verify

$$\tilde{X} = \begin{pmatrix} X & 0 \\ 0 & X \end{pmatrix}, \quad \tilde{Y} = \begin{pmatrix} Y & J^{1/2} \\ J^{1/2} & -Y \end{pmatrix}, \quad \tilde{W} = \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix}$$

is in $\widehat{\mathcal{D}_p}$. Since $J \neq 0$, the tuple (X, Y, W) is not a Euclidean extreme point of $\widehat{\mathcal{D}_p}$ by Theorem 1.1(1). Similarly, to conclude (X, Y) is not a Euclidean extreme point of $\mathcal{C}$ verify

$$\tilde{X} = \begin{pmatrix} X & 0 \\ 0 & X \end{pmatrix}, \quad \tilde{Y} = \begin{pmatrix} Y & J^{1/2} \\ J^{1/2} & -Y \end{pmatrix}$$

is in $\mathcal{C}$.

Finally, we prove the final assertion in the proposition. Suppose

$$\tilde{X} = \begin{pmatrix} X & \alpha \\ \alpha^* & * \end{pmatrix}, \quad \tilde{Y} = \begin{pmatrix} Y & \beta \\ \beta^* & Y_* \end{pmatrix}, \quad \tilde{W} = \begin{pmatrix} Y^2 & t \\ t^* & W_* \end{pmatrix}$$

is in $\widehat{\mathcal{D}_p}$. Then $I - \tilde{X}^2 - \tilde{S}^2 \succeq 0$ gives, in the top left corner, that $I - X^2 - \alpha\alpha^* - Y^4 - tt^* = -\alpha\alpha^* - tt^* \succeq 0$. Thus $\alpha = t = 0$. Additionally, $\tilde{W} \succeq \tilde{Y}^2$ gives that, examining the top left corner, $-\beta\beta^* \succeq 0$. Thus $\beta = 0$. Therefore $(X, Y, Y^2) \in \partial^{\mathrm{arv}}\widehat{\mathcal{D}_p}$.

Now suppose $\tilde{X}$ and $\tilde{Y}$ are given as in equation (7.7) and $(\tilde{X}, \tilde{Y}) \in \mathcal{C}$. There exists a $\tilde{S}$ as in equation (7.7) such that $(\tilde{X}, \tilde{Y}, \tilde{S})$ is in $\widehat{\mathcal{D}_p}$. Again, by observing the top left corners of the inequalities $I - \tilde{X}^2 - \tilde{S}^2 \succeq 0$ and $\tilde{S} \succeq \tilde{Y}^2$, it follows that $Y^4 - S^2 = I - X^2 - S^2 \succeq \alpha\alpha^* + tt^* \succeq 0$ and $S - Y^2 \succeq \beta\beta^* \succeq 0$. Since the square root function is matrix monotone, $Y^2 \succeq S \succeq Y^2$. Hence $S = Y^2$. Now $\beta = \alpha = 0$ from the first part of this proof and therefore $(X, Y) \in \partial^{\text{arv}}\mathcal{C}$. The final claim is a consequence of Proposition 3.7. ∎

7.3.4. *Proof of Proposition 7.8.* It suffices to show there is an (X, Y, W) satisfying the hypotheses of Proposition 7.10(1b). To show there are in fact many (X, Y, W) that satisfy the hypotheses of the lemma, choose a rank one positive J and a Y such that and $JY^2 + Y^2J - J^2$ is not positive semidefinite and $W = Y^2 + J$ is a contraction; i.e., $I - W^2 \succeq 0$. Choose X such that $X^2 = I - W^2$. Hence $(X, Y, W) \in \widehat{A}$. On the other hand, since

$$I - X^2 - Y^4 = JY^2 + Y^2J - J^2 \nsucceq 0,$$

$(X, Y) \notin \mathcal{D}_p$. It is easy to actually construct such X, Y, W. The choice

$$(7.9) \qquad Y = \sqrt{\mu}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \qquad W = \mu\begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \qquad X^2 = 1 - W^2.$$

with μ chosen so that the norm of W is 1 appears in [HKM16]. ∎

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Contents