MATRIX EXTREME VERSUS FREE EXTREME

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PREFACE

This honors thesis comes from an article that is being prepared for publication. The specific contributions of Aidan Epperly will be included in an appendix section at the end of the paper.

MATRIX EXTREME VERSUS FREE EXTREME

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ABSTRACT. A spectrahedron is a convex set defined to be the solution set of a linear matrix inequality, which is to say the set of all $x \in \mathbb{R}^g$ such that

$$L_A(x) = I + A_1x_1 + A_2x_2 + \cdots + A_gx_g \succeq 0.$$

This notion can be extended by instead taking X to be a tuple of real symmetric matrices of any size $n \times n$ using the Kronecker product

$$L_A(X) = I_n \otimes I_d + A_1 \otimes X_1 + A_2 \otimes X_2 + \cdots + A_g \otimes X_g$$

The solution set of $L_A(X) \succeq 0$ is called a *free spectrahedron*. Free spectrahedra play an important roll in systems engineering, operator algebra, and the theory of matrix convex sets. Matrix extreme points of free spectrahedra are of particular interest.

The results of this paper fall into three main categories: theoretical, algorithmic, and experimental. Firstly, we prove the existence of matrix extreme points of free spectrahedra that are not free extreme. This is done by producing exact arithmetic examples of matrix extreme points that are not free extreme. Secondly, we detail a number of methods for constructing matrix extreme points of free spectrahedra that are not free extreme, both exactly and approximately (numerically). We also show how a recent result due to Kriel, found in [K19], can be used to efficiently test whether a point is matrix extreme. Thirdly, we provide evidence, through a series of numerical experiments, that there are a substantial number of matrix extreme points of free spectrahedra that are not free extreme.

Contents

1. Introduction

1.1. **Matrix convex sets and free spectrahedra.** A matrix $B \in M_n(\mathbb{R})$ is said to be **positive semidefinite** if it is symmetric, i.e. $B = B^T$, and all of its eigenvalues are nonnegative. Let

$$B \succeq 0$$

denote that the matrix B is positive semidefinite. Similarly, given two symmetric matrices $B_1, B_2 \in M_{n\times n}(\mathbb{R})$, let

$$B_1 \succeq B_2$$

denote that $B_1 - B_2$ is positive semidefinite.

1.1.1. *Matrix Convex Sets.* Let $SM_n(\mathbb{R})^g$ denote the set of all g-tuples of real symmetric $n \times n$ matrices X_i and set $SM(\mathbb{R})^g = \cup_n SM_n(\mathbb{R})^g$. Similarly, we let $M_{m\times n}(\mathbb{R})^g$ denote the set of g-tuples of $m \times n$ matrices with real entries.

Given some finite collection $\{X^i\}_{i=1}^{\ell}$ with $X^i \in SM_{n_i}(\mathbb{R})^g$ for each $i = 1, 2, \ldots, \ell$, a **matrix convex combination** of $\{X^i\}_{i=1}^{\ell}$ is a sum of the form

$$\sum_{i=1}^{\ell} V_i^T X^i V_i \qquad \text{with} \quad \sum_{i=1}^{\ell} V_i^T V_i = I_n$$

where $V_i \in M_{n_i\times n}(\mathbb{R})$ and

$$V_i^T X^i V_i = \left(V_i^T X_1^i V_i, V_i^T X_2^i V_i, \ldots, V_i^T X_g^i V_i\right) \in SM_n(\mathbb{R})^g$$

for all $i = 1, 2, \ldots, \ell$. We emphasize that the tuples X^i need not be the same size. A matrix convex combination is called **proper** if V_i is surjective for all $i = 1, 2, \ldots, \ell$.

A set $\Gamma \subseteq SM(\mathbb{R})^g$ is **matrix convex** if it is closed under matrix convex combinations. The **matrix convex hull** of a set $\Gamma \subseteq SM(\mathbb{R})^g$ is the set of all matrix convex combinations of the elements of Γ. Equivalently, the matrix convex hull of $\Gamma \subseteq SM(\mathbb{R})^g$ is the smallest matrix convex set containing Γ. That is, Γ is the intersection of all matrix convex sets containing Γ.

A set $\Gamma \subseteq SM(\mathbb{R})^g$ is a **matrix cone** if given some finite collection $\{X^i\}_{i=1}^{\ell}$ with $X^i \in SM_{n_i}(\mathbb{R})^g$ for each $i = 1, 2, \ldots, \ell$ and $V_{n_i} \in M_{n_i\times n}(\mathbb{R})$, then

$$\sum_{i=1}^{\ell} V_i^T X^i V_i \in \Gamma.$$

1.2. **Free spectrahedra and linear matrix inequalities.** In this paper, we primarily concern ourselves with a specific class of matrix convex sets called free spectrahedra. A free spectrahedron is a matrix convex set which can be defined by a linear matrix inequality. Fix a tuple $A \in SM_d(\mathbb{R})^g$ of $d \times d$ symmetric matrices. A **monic linear pencil** $L_A(x)$ is a sum of the form

$$L_A(x) = I_d + A_1x_1 + A_2x_2 + \cdots + A_gx_g.$$

Given a tuple $X \in SM_n(\mathbb{R})^g$, the **evaluation** of L_A at X is

$$L_A(X) = I_d \otimes I_n + A_1 \otimes X_1 + A_2 \otimes X_2 + \cdots + A_g \otimes X_g$$

where $\otimes$ denotes the Kronecker Product. A **linear matrix inequality** is an inequality of the form

$$L_A(X) \succeq 0.$$

Let $\Lambda_A(X)$ denote the linear part of $L_A(X)$, i.e.

$$\Lambda_A(X) = A_1 \otimes X_1 + A_2 \otimes X_2 + \cdots + A_g \otimes X_g$$

so that $L_A(X) = I_{dn} + \Lambda_A(X)$.

Given a g-tuple $A \in SM_n(\mathbb{R})^g$ and a positive integer n, we define the **free spectrahedron $\mathcal{D}_A$ at level** n, denoted $\mathcal{D}_A(n)$, by

$$\mathcal{D}_A(n) := \{X \in SM_n(\mathbb{R})^g : L_A(X) \succeq 0\}.$$

That is, $\mathcal{D}_A(n)$ is the set of all g-tuples of $n \times n$ real symmetric matrices X such that the evaluation $L_A(X)$ is positive semidefinite. Defined the **free spectrahedron** $\mathcal{D}_A$ to be the union over all n of the free spectrahedron $\mathcal{D}_A$ at level n, i.e.

$$\mathcal{D}_A := \cup_{n=1}^{\infty} \mathcal{D}_A(n) \subseteq SM(\mathbb{R})^g.$$

Lemma 1.1. *Let $A \in SM_d(\mathbb{R})^g$ and let $\mathcal{D}_A$ the the associated free spectrahedron. Then $\mathcal{D}_A$ is matrix convex.*

Proof. The matrix convexity of free spectrahedra follows quickly from the fact that $I_{dn} + \Lambda_A(X) \succeq 0$ implies that $I_{dn} \otimes V^TV + \Lambda_A(V^TXV) \succeq 0$. ■

We say a free spectrahedron is **bounded** if there is some fixed real number C so that

$$CI_n - \sum_{i=1}^{g} X_i^2 \succeq 0$$

for all $X = (X_1, X_2, \ldots, X_g) \in \mathcal{D}_A$ and all positive integers n. It is routine to show that a free spectrahedron is bounded if and only if $\mathcal{D}_A(1)$ is bounded [HKM13]. In our definition of a free spectrahedron, we use a non-strict inequality. All free spectrahedra

defined in this way are closed in the sense that each $\mathcal{D}_A(n)$ is closed. Some authors do not use such a definition and thus consider free spectrahedra that are not closed.

1.2.1. *Homogeneous free spectrahedra.* It is occasionally useful to consider the homogeneous free spectrahedron. Given a tuple $A \in SM_d(\mathbb{R})^g$ the **homogeneous free spectrahedron $\mathcal{H}_A$ at level** n, denoted $\mathcal{H}_A(n)$, by

$$\mathcal{H}_A(n) := \left\{X \in SM_n(\mathbb{R})^{g+1} : \Lambda_A(X) \succeq 0\right\}$$

and the **homogeneous free spectrahedron $\mathcal{H}_A$** is defined as the union over all positive integers n of $\mathcal{H}_A(n)$, i.e.

$$\mathcal{H}_A = \cup_{n=1}^{\infty} \mathcal{H}_A(n) \subseteq SM(\mathbb{R})^g$$

1.3. **Extreme points of free spectrahedra.** The extreme points of matrix convex sets and free spectrahedra are of particular interest, since they have Krein-Milman type spanning properties. The paper will primarily consider three types of extreme points: Euclidean extreme points, matrix extreme points, and free extreme points.

Given a matrix convex set Γ, we say $X \in \Gamma(n)$ is a **Euclidean extreme point** of Γ if X cannot be written as a nontrivial classical convex combination of points in $\Gamma(n)$. We note that this is the same as being a classical extreme point of $\Gamma(n)$. We let $\partial^{\text{Euc}}\Gamma$ denote the set of all the Euclidean extreme points of Γ.

Two tuples $X, Z \in \Gamma(n)$ are said to be **unitarily equivalent** if there exists some unitary matrix U_j such that $X_j = U_j^T Z_j U_j$. We say a point $X \in \Gamma(n)$ is a **matrix extreme point** of Γ if whenever X is written as a proper matrix convex combination

$$X = \sum_{i=1}^{\ell} V_i^T X^i V_i \qquad \text{with} \quad \sum_{i=1}^{\ell} V_i^T V_i = I_n$$

of points $X^i \in \Gamma$ for $i = 1, 2, \ldots, \ell$, then for every $i = 1, 2, \ldots, \ell$, we have $V_i \in M_{n\times n}(\mathbb{R})$ and X is unitarily equivalent to X^i. We let $\partial^{\text{mat}}\Gamma$ denote the set of all the matrix extreme points of Γ.

Finally, we say a point $X \in \Gamma(n)$ is a **free extreme point** of Γ if whenever X is written as a matrix convex combination

$$X = \sum_{i=1}^{\ell} V_i^T X^i V_i \qquad \text{with} \quad \sum_{i=1}^{\ell} V_i^T V_i = I_n$$

of points $X^i \in \Gamma$ with $V_i \neq 0$ for each i, then for all $i = 1, 2, \ldots, \ell$ either $V_i \in M_{n\times n}(\mathbb{R})$ and X is unitarily equivalent to X^i or $V_i \in M_{n_i\times n}(\mathbb{R})$ where $n_i > n$ and there exists $Z^i \in \Gamma$ such that $X \oplus Z^i$ is unitarily equivalent to X^i. In words, a point X is a free

extreme point of Γ if it cannot be written as a nontrivial matrix convex combination of points in Γ. We let $\partial^{\text{free}}\Gamma$ denote the set of all the free extreme points of Γ.

1.3.1. *Irreducible matrix tuples.* Given a matrix $M \in M_{n\times n}(\mathbb{R})$, a subspace $N \subseteq \mathbb{R}^n$ is a **reducing subspace** if both N and $N^\perp$ are invariant subspaces of M, which is to say that N is a reducing subspace of M if $MN \subseteq N$ and $MN^\perp \subseteq N^\perp$. A tuple $X \in SM_n(\mathbb{R})^g$ is **irreducible** (over $\mathbb{R}$) if the matrices $X_1, \ldots, X_g$ have no common reducing subspaces in $\mathbb{R}^n$; a tuple is **reducible** (over $\mathbb{R}$) if it is not irreducible. Since we will always be working over $\mathbb{R}$ in this paper, we will drop the use of "over $\mathbb{R}$" and simply refer to tuples as reducible or irreducible.

Remark 1.2. *Given a matrix convex set Γ, if $X \in \Gamma$ is matrix extreme, then X is irreducible. This is proved over the complexes in* [EHKM18, Theorem 1.1 (2)]. *The proof over the reals is similar.*

1.4. **Significance of free and matrix extreme points.** The concept of matrix extreme points was introduced by Webster and Winkler in [WW99]. It is known that the matrix convex hull of the matrix extreme points of a matrix convex set Γ is equal to Γ [WW99, K19]. In particular, this means that every point in a free spectrahedron can be written as a matrix convex combination of matrix extreme points. It was later shown in [EH19] that a free spectrahedron $\mathcal{D}_A$ is the matrix convex hull of it's free extreme points. Moreover, the free extreme points are the smallest set with this property.

Theorem 1.3 ([EH19, Theorem 1.1])**.** *Let $A \in SM_d(\mathbb{R})^g$ such that $\mathcal{D}_A$ is a bounded free spectrahedron. Then $\mathcal{D}_A$ is the matrix convex hull of its free extreme points. Furthermore, if $E \subseteq \mathcal{D}_A$ is a set of irreducible tuples which is closed under unitary equivalence and whose matrix convex hull is equal to $\mathcal{D}_A$, then E must contain the free extreme points of $\mathcal{D}_A$.*

Thus, the free extreme points are, in some sense, the correct notion of extreme points for free spectrahedra. Moreover, the set of all free extreme points of a free spectrahedron must be contained in the set of all matrix extreme points.

1.5. **Main Results.** The results of this paper fall into three main categories: theoretical, algorithmic, and experimental. Firstly, we show the existence of matrix extreme points of free spectrahedra that are not free extreme, thus proving that the containment of free extreme points within matrix extreme points is, in some cases, strict. This is done by producing exact arithmetic examples of matrix extreme points that are not free extreme. Secondly, we detail a number of methods for constructing

matrix extreme points of free spectrahedra that are not free extreme, both exactly and numerically. We also show how a recent result due to Kriel, found in [K19], can be used to efficiently test whether a point is matrix extreme. Thirdly, we provide evidence, through a series of numerical experiments, that there are a substantial number of matrix extreme points of free spectrahedra that are not free extreme.

The paper is organized as follows. Section 2 focuses on the background theory underpinning our results. Of note is Theorem 2.2, a result of Kriel [K19], which allows us to characterize matrix extreme points. In Section 3 we exhibit examples of tuples that are matrix extreme points but not free extreme. Section 4 and Section 5 describe algorithms for generating numerical and exact extreme points respectively. Section 4 focuses heavily on empirical observations resulting from a number of numerical experiments; that leads us to believe that MnotA extreme points are not rare. Section 5 shows how a similar approach to that used in Section 4 can be modified to produce matrix extreme points using exact arithmetic.

2. Background Theory

2.1. **Minimal Defining Tuples.** Throughout this paper, the size of the defining tuple of a free spectrahedron will play an important role in our analysis. However, we must note that the defining tuple of a free spectrahedron is not unique. For instance, $A \in SM_d(\mathbb{R})^g$ and $A \oplus A$ both define the same free spectrahedron despite $A \oplus A$ being in $SM_{2d}(\mathbb{R})^g$. Thus, we would not necessarily expect the size of the defining tuple of a spectrahedron to be an inherent property of the free spectrahedron. We can, however, overcome this with the concept of a **minimal defining tuple**. Using [HKM13, Theorem 3.12 and Corollary 3.18], we can define a minimal defining tuple $\widetilde{A} \in SM_d(\mathbb{R})^g$ of a free spectrahedron $\mathcal{D}_A$ as a tuple of minimal size such that $\mathcal{D}_{\widetilde{A}} = \mathcal{D}_A$. That is to say if $\widetilde{A} \in SM_d(\mathbb{R})^g$ is a minimal defining tuple of $\mathcal{D}_A$ then if $\hat{A} \in SM_n(\mathbb{R})^g$ for $n < d$, $\mathcal{D}_{\hat{A}} \neq \mathcal{D}_{\widetilde{A}}$. Throughout the rest of the paper, we will always assume that the defining tuple of a free spectrahedron is minimal.

2.2. **Characterizing Extreme Points.** An important class of extreme points that has yet to be discussed is the **Arveson extreme points** which arise from dilation theory. A point $X \in \Gamma$ is an Arveson extreme point of Γ if

$$Y = \begin{pmatrix} X & \beta \\ \beta^T & \gamma \end{pmatrix} \in \Gamma$$

implies $\beta = 0$ for $\beta \in M_{n\times 1}(\mathbb{R})^g$. We can also provide a similar definition of a Euclidean extreme point in the language of dilation theory using the following proposition.

Proposition 2.1 ([EHKM18, Corollary 2.3]). *A point X in a free spectrahedron $\mathcal{D}_A$ is a Euclidean extreme point of $\mathcal{D}_A$ if and only if*

$$Y = \begin{pmatrix} X & \beta \\ \beta & \gamma \end{pmatrix} \in \mathcal{D}_A$$

implies $\beta = 0$ for $\beta \in SM_n(\mathbb{R})^g$.

A theorem of Kriel gives a similarly nice result regarding matrix extreme points.

Theorem 2.2 ([K19, Theorem 6.5.c]). *A point X in a bounded free spectrahedron $\mathcal{D}_A$ is a matrix extreme point of $\mathcal{D}_A$ if and only if (I, X) is on a classical extreme ray of $\mathcal{H}_{(I,A)}$.*

Proof. For the forward direction, suppose $X \in \mathcal{D}_A(n)$ is a matrix extreme point of the bounded free spectrahedron $\mathcal{D}_A$. By [E21, Lemma 2.2] and [K19, Theorem 6.5.b] every element of $\mathcal{H}_{(I,A)}(k)$ can be written in the form (V^TV, V^TYV) for $Y \in \mathcal{D}_A(k_0)$ and $V \in M_{k_0\times k}(\mathbb{R})$ surjective. For $i = 1, 2, \ldots, m$, fix $Y^i \in \mathcal{D}_A(n_i)$, $V_i \in M_{n_i\times n}(\mathbb{R})$ surjective, $\alpha_i > 0$ such that

$$(I, X) = \sum_{i=1}^m \alpha_i (V_i^T V_i, V_i^T Y^i V_i)$$

and $(V_i^T V_i, V_i^T Y^i V_i) \in \mathcal{H}_{(I,A)}$. Letting $U_i = \sqrt{\alpha_i} V_i$, we get

$$(I, X) = \sum_{i=1}^m (U_i^T U_i, U_i^T Y^i U_i) = (\sum_{i=1}^m U_i^T U_i, \sum_{i=1}^m U_i^T Y^i U_i),$$

and thus $X = \sum_{i=1}^m U_i^T Y^i U_i$ is a proper convex combination. Since X is assumed to be matrix extreme, $n_i = n$ and there is $W_i \in M_{n\times n}(\mathbb{R})$ unitary and $\lambda_i > 0$ such that $X = W_i^T Y^i W_i$ and $U_i = \lambda_i W_i$ for $i = 1, 2, \ldots, m$. So $(V_i^T V_i, V_i^T Y^i V_i)$ is a scalar multiple of (I, X).

For the reverse direction, suppose $X \in \mathcal{D}_A(n)$ such that (I, X) is on a classical extreme ray of $\mathcal{H}_{(I,A)}$ and there are $Y^i \in \mathcal{D}_A(n_i)$ and $V_i \in M_{n_i\times n}$ surjective for $i = 1, 2, \ldots, m$ with $I = \sum_{i=1}^m V_i^T V_i$ and $X = \sum_{i=1}^m V_i^T Y^i V_i$. Without loss of generality we may assume $n_i = n$ by replacing Y^i with $Y^i \oplus 0$. Thus

$$(I, X) = (\sum_{i=1}^m V_i^T V_i, \sum_{i=1}^m V_i^T Y^i V_i) = \sum_{i=1}^m (V_i^T V_i, V_i^T Y^i V_i).$$

As (I, X) is on a classical extreme ray, $(V_i^T V_i, V_i^T Y^i V_i) = \alpha_i(I, X)$ for some $\alpha_i > 0$. In particular $V_i^T V_i = \alpha_i I$, so $W_i = (\alpha_i^{-\frac{1}{2}})V_i$ is unitary, V_i is surjective, and X is unitarily equivalent to Y^i for $i = 1, 2, \ldots, m$. ■

Corollary 2.3. *If a point X is in a bounded free spectrahedron $\mathcal{D}_A$, then the following are equivalent*

(1) X is a matrix extreme point of $\mathcal{D}_A$
(2) (I, X) is on an classical extreme ray of $\mathcal{H}_{(I,A)}$
(3) $(\beta_0, \beta) \in SM_n(\mathbb{R})^{g+1}$ and

$$\ker \Lambda_{(I,A)}(I, X) \subseteq \ker \Lambda_{(I,A)}((\beta_0, \beta)) \implies (\beta_0, \beta) \in \operatorname{span}((I, X))$$

(4) For $(\beta_0, \beta), (\gamma_0, \gamma) \in SM_n(\mathbb{R})^{g+1}$

$$(Y_0, Y) = \begin{pmatrix} (I, X) & (\beta_0, \beta) \\ (\beta_0, \beta) & (\gamma_0, \gamma) \end{pmatrix} \in \mathcal{H}_{(I,A)}$$

implies $(\beta_0, \beta) \in \operatorname{span}((I, X))$.

Proof. The equivalence of Item 1 and Item 2 follows from Theorem 2.2. The equivalence of Item 2 and Item 3 is [RG95, Corollary 4] by viewing (I, X) as an element of $\mathbb{R}^{\frac{n(n+1)(g+1)}{2}}$.

To show the equivalence of Item 3 and Item 4, let $(\beta_0, \beta), (\gamma_0, \gamma) \in SM_n(\mathbb{R})^{g+1}$ such that

$$(Y_0, Y) = \begin{pmatrix} (I, X) & (\beta_0, \beta) \\ (\beta_0, \beta) & (\gamma_0, \gamma) \end{pmatrix}$$

By conjugating by permutation matrices, sometimes called canonical shuffles, we can show that $\Lambda_{(I,A)}((Y_0, Y))$ is unitarily equivalent to

$$\begin{pmatrix} \Lambda_{(I,A)}((I, X)) & \Lambda_{(I,A)}((\beta_0, \beta)) \\ \Lambda_{(I,A)}((\beta_0, \beta)) & \Lambda_{(I,A)}((\gamma_0, \gamma)) \end{pmatrix}. \tag{2.1}$$

A routine calculation using the above then shows that if $(Y_0, Y) \in \mathcal{H}_{(I,A)}$ implies

$$\ker \Lambda_{(I,A)}((I, X)) \subseteq \ker \Lambda_{(I,A)}((\beta_0, \beta)).$$

It follows that Item 3 implies Item 4.

Now assume that Item 4 holds. Taking the Schur complement the matrix in Equation (2.1) shows that $\Lambda_{(I,A)}((Y_0, Y)) \succeq 0$ if and only if

$$\Lambda_{(I,A)}((I, X)) - \Lambda_{(I,A)}((\beta_0, \beta))(\Lambda_{(I,A)}((\gamma_0, \gamma)))^\dagger \Lambda_{(I,A)}((\beta_0, \beta)) \succeq 0 \tag{2.2}$$

and

$$\Lambda_{(I,A)}((\gamma_0,\gamma)) \succeq 0 \tag{2.3}$$

where † denotes the Moore-Penrose pseudoinverse. Fix $(Z_0, Z) \in SM_n(\mathbb{R})^{g+1}$ such that

$$\ker \Lambda_{(I,A)}((I,X)) \subseteq \ker \Lambda_{(I,A)}((Z_0,Z)).$$

Then, considering equations Equation (2.2) and Equation (2.3) shows that there is some $\alpha > 0$ such that for $(\gamma_0,\gamma) = (I,0)$ and $(\beta_0,\beta) = \alpha(Z_0,Z)$ we have $(Y_0,Y) \in \mathcal{H}_{(I,A)}$. By assumption, (β_0,β) must be in the span of (I,X) and thus, (Z_0,Z) is too. ■

Using these characterizations of Euclidean and matrix extreme points, we can arrive at the following known result, see [EHKM18, Theorem 1.1].

Proposition 2.4. *Let $\mathcal{D}_A$ be a bounded free spectrahedron.*

1. *A tuple X is a free extreme point of $\mathcal{D}_A$ if and only if X is an irreducible Arveson extreme point of $\mathcal{D}_A$.*
2. *If a tuple X is a free extreme point of $\mathcal{D}_A$, then X is a matrix extreme point of $\mathcal{D}_A$.*
3. *If a tuple X is a matrix extreme point of $\mathcal{D}_A$, then X is a Euclidean extreme point of $\mathcal{D}_A$.*
4. *If a tuple X is an Arveson extreme point of $\mathcal{D}_A$, then X is a Euclidean extreme point of $\mathcal{D}_A$.*

Proof. Item 1 and Item 4 are the subject of [EHKM18, Theorem 1.1], where the proof is given working over $\mathbb{C}$. The proof of Item 4 can be used over $\mathbb{R}$ without modification, and the proof of Item 1 over $\mathbb{R}$ is given by [EH19, Theorem 1.2]. Item 2 follows from [EH19, Theorem 1.1] which is given as Theorem 1.3 here. Item 3 follows from the observation that if X can be written as a nontrivial classical convex combination $X = \alpha_1 X^1 + \alpha_2 X^2 + \cdots + \alpha_\ell X^\ell$, then $(I,X) = \alpha_1(I,X^1) + \alpha_2(I,X^2) + \cdots + \alpha_\ell(I,X^\ell)$ is a nontrivial classical convex combination of points in $\mathcal{H}_{(I,A)}$. ■

From this proposition, we get the following corollary immediately.

Corollary 2.5. *Let $\mathcal{D}_A$ be a bounded free spectrahedron. If X is a matrix extreme point of $\mathcal{D}_A$, then X is a free extreme point of $\mathcal{D}_A$ if and only if X is an Arveson extreme point of $\mathcal{D}_A$.*

Proof. A point in $\mathcal{D}_A$ is free extreme if and only if it is irreducible and Arveson extreme. If X is a matrix extreme point of $\mathcal{D}_A$, then in particular X is irreducible and thus X is free extreme if and only if X is Arveson extreme. ■

Thus, if X is a matrix extreme point of $\mathcal{D}_A$, to show that X is not free extreme it is sufficient to show it is not Arveson extreme. This result is particularly important as it is computationally easier to determine if a point is Arveson extreme than to show it is free extreme. This is because checking if a tuple is Arveson extreme is straightforward, indeed it is equivalent to solving the upcoming linear system Equation (2.4). For this reason, we will refer to the set of matrix extreme points that are not free extreme points as MnotA extreme.

2.2.1. *Extreme points and linear systems.* It is possible to determine if a point X in the free spectrahedron $\mathcal{D}_A$ is extreme by solving a linear system. Given a free spectrahedron $\mathcal{D}_A$ and a point $X \in \mathcal{D}_A$ we let

$$k_{A,X} := \dim \ker L_A(X)$$

and let $K_{A,X} : \mathbb{R}^{nd} \to \mathbb{R}^{k_{A,X}}$ be a matrix who's columns form an orthonormal basis for the kernel of $L_A(X)$.

Proposition 2.6. *Let $\mathcal{D}_A$ be a bounded free spectrahedron and $X \in \mathcal{D}_A(n)$.*

(1) X is an Arveson extreme point of $\mathcal{D}_A$ if and only if the only solution to the homogeneous linear equations

$$\Lambda_A(\beta^T)K_{A,X} = (A_1 \otimes \beta_1^T + \cdots + A_n \otimes \beta_g^T)K_{A,X} = 0 \tag{2.4}$$

in the unknown $\beta \in M_{n\times 1}(\mathbb{R})^g$ is $\beta = 0$.

(2) X is a Euclidean extreme point of $\mathcal{D}_A$ if and only if the only solution to the homogeneous linear equations

$$\Lambda_A(\beta)K_{A,X} = (A_1 \otimes \beta_1 + \cdots + A_n \otimes \beta_g)K_{A,X} = 0 \tag{2.5}$$

in the unknown $\beta \in SM_n(\mathbb{R})^g$ is $\beta = 0$.

(3) X is a matrix extreme point of $\mathcal{D}_A$ if and only if the only solution to the homogeneous linear equations

$$\Lambda_{(I,A)}(\beta_0, \beta)K_{A,X} = (I \otimes \beta_0 + A_1 \otimes \beta_1 + \cdots + A_n \otimes \beta_g)K_{A,X} = 0 \tag{2.6}$$

$$\langle (I, X), (\beta_0, \beta) \rangle = \operatorname{tr}(\beta_0 + X_1^T\beta_1 + \cdots + X_g^T\beta_g) = 0 \tag{2.7}$$

in the unknown $(\beta_0, \beta) \in SM_n(\mathbb{R})^{g+1}$ is $\beta = 0$.

Proof. The proofs for each of the above results are all quite similar, so details of the proofs for Item 1 and Item 2 will be omitted.

The assertion given in Item 1 regarding Arveson extreme points is the content of [EH19, Lemma 2.1 (3)]. It is due to Evert and Helton.

The assertion given in Item 2 regarding Euclidean extreme points is the content of [EHKM18, Corollary 2.3]. It follows from [RG95, Corollary 3] which is due to Ramana and Goldman.

To show Item 3, we note that by Theorem 2.2 and Corollary 2.3 X is matrix extreme if and only if for $(\beta_0, \beta), (\gamma_0, \gamma) \in SM_n(\mathbb{R})^{g+1}$

$$(Y_0, Y) = \begin{pmatrix} (I, X) & (\beta_0, \beta) \\ (\beta_0, \beta) & (\gamma_0, \gamma) \end{pmatrix} \in \mathcal{H}_{(I,A)}$$

implies $(\beta_0, \beta) \in \operatorname{span}((I, X))$.

Clearly $\ker \Lambda_{(I,A)}((I, X)) = \ker L_A(X)$ so $K_{A,X}$ is a matrix whose columns form an orthonormal basis of $\ker \Lambda_{(I,A)}((I, X))$ as well. If there is a (β_0, β) such that $(Y_0, Y) \in \mathcal{H}_{(I,A)}$ and (β_0, β) is not in the span of (I, X), then by Equation (2.3) it follows that

$$\ker \Lambda_{(I,A)}((I, X)) \subseteq \ker \Lambda_{(I,A)}((\beta_0, \beta)).$$

We can write $(\beta_0, \beta) = (\beta_0', \beta') + \alpha(I, X)$ for $\alpha \in \mathbb{R}$ and $(\beta_0', \beta') \neq 0$ satisfying Equation (2.7). The containment

$$\ker \Lambda_{(I,A)}((I, X)) \subseteq \ker \Lambda_{(I,A)}((\beta_0, \beta)) = \ker(\Lambda_{(I,A)}(\alpha(I, X)) + \Lambda_{(I,A)}((\beta_0', \beta')))$$

implies that

$$\ker \Lambda_{(I,A)}((I, X)) \subseteq \ker \Lambda_{(I,A)}((\beta_0', \beta')).$$

Hence, there is a nonzero (β_0', β') satisfying Equation (2.6) and Equation (2.7).

Conversely, if there is (β_0, β) satisfying Equation (2.6) and Equation (2.7), then by taking $(\gamma_0, \gamma) = (I, 0)$ the argument above reverses to show X is not matrix extreme. ■

We can use Proposition 2.6 to obtain the following corollary.

Corollary 2.7. *Let $A \in SM_d(\mathbb{R})^g$ be a minimal defining tuple for $\mathcal{D}_A$ and let $X \in \mathcal{D}_A(n)$. We define $k_{A,X} = \ker L_A(X)$. Then,*

(1) if X is Arveson extreme then

$$gn \leq dk_{A,X} \tag{2.8}$$

(2) if X is Euclidean extreme then

$$\frac{g(n+1)}{2} \leq dk_{A,X} \tag{2.9}$$

(3) if X is matrix extreme then

$$\frac{n(n+1)(g+1)}{2} \leq dnk_{A,X} + 1 \tag{2.10}$$

where $k_{A,X}$ is the dimension of the kernel of $L_A(X)$.

For brevity, we will often refer to

(1) $\left\lceil \frac{gn}{d} \right\rceil$ as the Arveson extreme equation count
(2) $\left\lceil \frac{g(n+1)}{2d} \right\rceil$ as the Euclidean extreme equation count
(3) $\left\lceil \frac{(n+1)(g+1)}{2d} - \frac{1}{nd} \right\rceil$ as the matrix extreme equation count.

In this terminology, for X to be a certain type of extreme point, the kernel dimension $k_{A,X}$ must be at least as large as the corresponding extreme equation count.

Proof. The above inequalities result from comparing number of equations to number of unknowns in the homogeneous linear equations given in Proposition 2.6. As an example the proof for Item 3 will be given below.

Equation (2.6) and Equation (2.7) are a set of homogeneous linear equations in the unknown $\beta \in SM_n(\mathbb{R})^{g+1}$. The matrix β has $n(n+1)(g+1)/2$ scalar unknowns so Equation (2.6) and Equation (2.7) can be written in the form $M\beta' = 0$ where

$$\beta = \left(\begin{pmatrix} \beta_{011} & \beta_{012} & \cdots & \beta_{01n} \\ \beta_{012} & \beta_{022} & \cdots & \beta_{02n} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{01n} & \beta_{02n} & \cdots & \beta_{0nn} \end{pmatrix}, \begin{pmatrix} \beta_{111} & \beta_{112} & \cdots & \beta_{11n} \\ \beta_{112} & \beta_{122} & \cdots & \beta_{12n} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{11n} & \beta_{12n} & \cdots & \beta_{1nn} \end{pmatrix}, \ldots, \begin{pmatrix} \beta_{g11} & \beta_{g12} & \cdots & \beta_{g1n} \\ \beta_{g12} & \beta_{g22} & \cdots & \beta_{g2n} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{g1n} & \beta_{g2n} & \cdots & \beta_{gnn} \end{pmatrix} \right)$$

$$\beta' = (\beta'_0, \beta'_1, \cdots, \beta'_n) \in \mathbb{R}^{\frac{n(n+1)(g+1)}{2}}$$

$$\beta'_i = (\beta_{i11}, \beta_{i12}, \cdots, \beta_{i1n}, \beta_{i22}, \beta_{i23}, \cdots, \beta_{i2n}, \beta_{i33}, \cdots, \beta_{inn})$$

and $M \in M_{dnk_{A,X}+1 \times \frac{n(n+1)(g+1)}{2}}(\mathbb{R})$ (Equation (2.6) has $dnk_{A,X}$ equations and Equation (2.7) is one). By the rank-nullity theorem, M has a nontrivial null space and thus there is a nontrivial β solving Equation (2.6) and Equation (2.7) if and only if

$$\frac{n(n+1)(g+1)}{2} > dnk_{A,X} + 1 \iff \left\lceil \frac{(n+1)(g+1)}{2d} - \frac{1}{nd} \right\rceil > k_{A,X}.$$

So if Equation (2.10) holds, M has a trivial null space and the only β solving Equation (2.6) and Equation (2.7) is $\beta = 0$. Hence by Proposition 2.6 X is not matrix extreme. ■

Lemma 2.8. *Let $A \in SM_n(\mathbb{R})^g$. If $g \geq n(n+1)/2$, then $\mathcal{D}_A$ is not bounded and $\mathcal{D}_A$ is not the matrix convex hull of its Arv/Euc/Mat extreme points. Furthermore, if $g > n(n+1)/2$ then $\mathcal{D}_A$ has no extreme points.*

Proof. Note that $\dim(SM_d(\mathbb{R})) = d(d+1)/2$. Using this it is straightforward to show that the span of $A_1, \ldots, A_g$ must contain a positive semidefinite matrix, hence $\mathcal{D}_A$ is not bounded and is not the matrix convex hull of its extreme points.

Now suppose $g > d(d+1)/2$. In this case there must exist $(\alpha_1, \alpha_2, \ldots, \alpha_g) \in \mathbb{R}^g$ such that $\sum \alpha_i A_i = 0$. A straightforward check shows that for any $X = (X_1, \ldots, X_g) \in \mathcal{D}_A$ one has $(X_1 + \gamma\alpha_1 I_n, \ldots, X_g + \gamma\alpha_g I_n) \in \mathcal{D}_A$ for all $\gamma \in \mathbb{R}$, hence X cannot be extreme.

■

3. Exact Points

To prove an example has our claimed properties, numerical calculations will not suffice due to the presence of some numerical error. However, usually it is difficult to find extreme points of free spectrahedra with exact arithmetic. Even in the smallest nontrivial case where the defining tuple $A \in SM_2(\mathbb{R})^2$ and the desired extreme point $X \in \mathcal{D}_A(2)$, exactly computing X by optimizing a linear functional requires computing an exact arithmetic solution to a semidefinite program with six variables and the constraint $L_A(X) \succeq 0$ where $L_A(X) \in SM_4(\mathbb{R})$. If the size of the defining tuple or the extreme point is greater than two, then computing even just a boundary point would require finding an exact solution to $\det(L_A(X)) = 0$, a polynomial equation of degree greater than five which is often impossible. For this reason, in a majority of cases, we opt to compute numerical extreme points instead of exact arithmetic extreme points. However, for some values of g, we do have exact arithmetic examples of MnotA extreme points which we exhibit here.

3.1. $g = 3$ MnotA extreme example.

Now we give an example for $g = 3$ of a bounded free spectrahedron $\mathcal{D}_A$ and a MnotA extreme point Y in it. In this case, A and Y have entries which are algebraic numbers and we have proved using exact arithmetic that Y is in $\mathcal{D}_A$ and is not Arveson extreme. To prove that Y is not matrix extreme one only needs to check that the Matrix Extreme Equation (2.6) has no solution. This we proved via floating point arithmetic by checking that the appropriate matrix has smallest singular value equal to 0.0318244 while largest singular value is not very large (< 5), hence it has no null space. In principle, one could prove this

using exact arithmetic, but after running the example for a while we stopped as exact arithmetic is not essential for the proof.

Now we state our example. Let

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

be the defining tuple of the free spectrahedron $\mathcal{D}_A$ and

$$Y = \left(\begin{pmatrix} \frac{1}{4} & \frac{27}{100} & b \\ \frac{27}{100} & -\frac{13}{100} & b \\ b & b & 0 \end{pmatrix}, \begin{pmatrix} -\frac{27}{100} & \frac{21}{100} & 3b \\ \frac{21}{100} & \frac{7}{100} & b \\ 3b & b & 0 \end{pmatrix}, \begin{pmatrix} \frac{7}{50} & -\frac{49}{100} & 3b \\ -\frac{49}{100} & \frac{3}{10} & 0 \\ 3b & 0 & 0 \end{pmatrix} \right)$$

where b is the smallest positive root of the polynomial

$$\begin{aligned} p_1(t) =& 20828330523 - 3649588559100t^2 + 132250437590000t^4 \\ & - 651404153000000t^6 + 748026200000000t^8. \end{aligned}$$

Then Y is a MnotA extreme point of $\mathcal{D}_A$. We know that p has a positive real zero as $p_1(0) = 20828330523$ and $p_1(\frac{1}{8}) = -\frac{208047637414661}{32768}$. So by the intermediate value theorem, there must be a zero between 0 and $\frac{1}{8}$. We go into detail on how this point was computed and proved to be a non-Arveson extreme point of $\mathcal{D}_A$ in Section 5.

3.2. **Exact arithmetic MnotA extreme point for $g = 4$.** For $g = 4$, we have an exact arithmetic example of a MnotA extreme point. Let $A = (A_1, A_2, A_3, A_4)$ for

$$A_1 = \operatorname{diag}\left(2, 0, -4, 0, 0, 0, -4, 0, \frac{8}{3}\right), \qquad A_2 = \operatorname{diag}\left(0, 4, -4, 0, 0, 0, 0, -\frac{8}{3}, \frac{8}{3}\right)$$
$$A_3 = \operatorname{diag}\left(0, 0, 0, 4, 0, -\frac{8}{3}, -4, 0, \frac{8}{3}\right), \qquad A_4 = \operatorname{diag}\left(0, 0, 0, 0, \frac{8}{3}, -\frac{8}{3}, 0, -\frac{8}{3}, \frac{8}{3}\right)$$

where $\mathrm{diag}(v)$ is the diagonal matrix whose diagonal is the vector v, be the defining tuple of the free spectrahedron $\mathcal{D}_A$. Then the tuple $X = (X_1, X_2, X_3, X_4)$ for

$$X_1 = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & \frac{3}{10} \end{pmatrix}$$

$$X_2 = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{\frac{3}{5}}}{4} \\ \frac{\sqrt{\frac{3}{5}}}{4} & -\frac{1}{5} \end{pmatrix}$$

$$X_3 = \begin{pmatrix} \frac{1521520\sqrt{3}-619599\sqrt{182}}{1019200\sqrt{3}-1197204\sqrt{182}} & 0 \\ 0 & -\frac{1}{4} \end{pmatrix}$$

$$X_4 = \begin{pmatrix} \frac{5\left(1664\sqrt{546}-124455\right)}{3143688} & -\frac{4\left(1820\sqrt{15}+669\sqrt{910}\right)}{392961} \\ -\frac{4\left(1820\sqrt{15}+669\sqrt{910}\right)}{392961} & \frac{11200\sqrt{546}-429603}{3143688} \end{pmatrix}$$

is a MnotA extreme point of $\mathcal{D}_A$.

The tuple X was computed by first taking an interior point of $\mathcal{D}_A$ with rational entries, and then perturbing each entry in order increase the kernel dimension $k_{A,X}$ to a suitable size. We can see the result of this method in the structure of X, as each of the X_i's is progressively more complicated.

Of note in this example is that the defining tuple A is a tuple of diagonal matrices, and thus $\mathcal{D}_A$ is a polytope.

4. How Common Are Matrix Extreme Points?

While there exist points that are MnotA extreme for free spectrahedra in $SM_n(\mathbb{R})^3$ and $SM_n(\mathbb{R})^4$, as demonstrated in Section 3, there is still the question of how frequently these points occur. To answer this question, we turn from methods of generating exact arithmetic extreme points to generating extreme points numerically. Numerical testing is an effective way of generating and testing a large number of points relatively quickly in order to get an idea (without proof) of whether or not example points are rare.

The most obvious method of generating an extreme point of a free spectrahedron $\mathcal{D}_A$ would be to optimize a random linear functional $\ell(X)$ under the constraint $L_A(X) \succeq 0$. However, in practice a surprisingly large majority of points generated by this method are Arveson extreme and have large $k_{A,X}$, as shown in [EFHY21]. Intuitively, and in fact empirically, we expect that points with large $k_{A,X}$ are more likely to be Arveson extreme. This intuition is based on the result given in Corollary 2.7.

As such, we wish to employ a method of generating extreme points that yields points with small kernels.

4.1. **Extreme Point Generation.** In the experiments detailed below, we will employ the following algorithm for numerical extreme point generation.

Algorithm 4.1. *Let $A \in SM_d(\mathbb{R})^g$ such that $\mathcal{D}_A$ is a bounded real free spectrahedron. Given an interior point $X \in \mathcal{D}_A(n)$, set $Y^0 = \frac{1}{1-\lambda}X$, where λ is the smallest eigenvalue of $L_A(X)$. If $\lambda = 1$, we instead pick some $\delta < 1$ and take $Y^0 = \frac{1}{1-\lambda_\delta}\delta X$ where λ_δ is the smallest eigenvalues of $L_A(\delta X)$. This multiplication guarantees Y^0 is a boundary point of $\mathcal{D}_A(n)$. For integers $j = 0, 1, 2, \ldots$ such that Y^j is neither an Arveson extreme point of $\mathcal{D}_A$ nor a matrix extreme point of $\mathcal{D}_A$, define*

$$Y^{j+1} := \begin{pmatrix} Y^j & c_j\hat{\beta}^j \\ c_j(\hat{\beta}^j)^T & \hat{\gamma}^j \end{pmatrix}$$

where $\hat{\beta}^j$ is a nonzero solution to

$$\ker L_A(Y^j) \subseteq \ker \Lambda_A(\beta^T), \quad \beta \in M_{n\times 1}(\mathbb{R})^g$$

and where c_j and $\hat{\gamma}^j$ are solutions to the sequence of maximization problems

$$\begin{aligned} c_j := \quad & \underset{c\in\mathbb{R},\gamma\in\mathbb{R}^g}{\text{Maximizer}} \quad c \\ & \text{s.t.} \quad L_A\begin{pmatrix} Y^j & c\hat{\beta}^j \\ c(\hat{\beta}^j)^T & \gamma \end{pmatrix} \succeq 0 \\ \text{and} \quad \hat{\gamma}^j := \quad & \underset{\gamma\in\mathbb{R}^g}{\text{Maximizer}} \quad \ell(\gamma) \\ & \text{s.t.} \quad L_A\begin{pmatrix} Y^j & c_j\hat{\beta}^j \\ c_j(\hat{\beta}^j)^T & \gamma \end{pmatrix} \succeq 0. \end{aligned}$$

Here ℓ is a random linear functional mapping $\mathbb{R}^g$ to $\mathbb{R}$.

Theorem 4.2. *Let $\mathcal{D}_A$ be a bounded free spectrahedron and let $X \in \mathcal{D}_A$. Then, with probability 1 Algorithm 4.1 terminates after some finite number k many steps and Y^k is either a matrix extreme or Arveson extreme point of $\mathcal{D}_A$.*

Proof. Algorithm 4.1 is almost identical to the dilation algorithm discussed in [EFHY21, Proposition 2.8] with the primary difference between the two algorithms being the construction of the initial point and the termination of Algorithm 4.1 in the case that some Y^i is matrix extreme. Thus, [EFHY21, Proposition 2.8] provides a finite upper bound on the number of steps that Algorithm 4.1 can take.

Moreover, if Algorithm 4.1 terminates after k steps, then either Y^k is matrix extreme or Y^k is Arveson extreme as these are the only conditions under which the algorithm terminates. ■

Given some Y^j as above, Y^{j+1} can be computed by solving two semidefinite programs. The first optimization computes the c_{j+1} and the second computes the $\hat{\gamma}^{j+1}$. These semidefinite programs can then be solved numerically. The introduction of numerical error into the problem requires some consideration. The first main consideration it that a given dilation step can fail in the sense that the dilation is not a maximal 1 dilation. In this case, we discard this failed dilation step and try again with a different β^{j+1}. The β^{j+1} in question is chosen by first computing a basis for the space of all β such that $\ker(L_A(Y^{j+1})) \subseteq \ker(\Lambda_A(\beta^T)$ and then taking a random convex combination of the basis vectors. Thus unless this space is one dimensional, we expect with probability 1 that the newly generated β^{j+1} will not be a scalar multiple of the original.

In order to prevent an infinite loop, we impose a limit on the number of failed dilation attempts on a single point to some maximum number. For the experiments below, this maximum was taken to be ten, meaning a point could fail to dilate ten times before the process was aborted. This number was chosen to be low as the importance of any particular point out of 10,000 trials is relatively low. In cases where it is important to dilate a particular point of interest to an Arveson or matrix extreme points, it may be appropriate to take a maximum which is much higher.

Another aspect of the algorithm is that there is a $\gamma \in SM_1(\mathbb{R})^g$ that is generated when we compute c_{j+1}, but this γ is "thrown out" and replaced with $\hat{\gamma}_{j+1}$ in the Y^{j+1}. In our experiments described below, we omit this second step and keep the original γ. Importantly, Theorem 4.2 does not guarantee the termination of this modified algorithm, but in practice it has been shown to be effective.

Given a bounded free spectrahedron $\mathcal{D}_A$, we can use Algorithm 4.1 to generate many extreme points $X \in \mathcal{D}_A(n)$ such that $k_{A,X}$ is relatively small. By producing a large number of extreme points in such a manner and then counting the number of MnotA extreme points, we can get a sense for how common such extreme points are.

4.1.1. *What Do We Call Zero?* There is another issue resulting from the introduction of numerical error, namely, what does it mean for a point X with floating point entries to be an extreme point. We can think of such an X as a sum $X = \widehat{X} + X_\delta$ where $\widehat{X}$ is an extreme point of $\mathcal{D}_A$ and X_δ as some small, nonzero error term. Such an X may not even be in $\mathcal{D}_A$, and is likely not an extreme point. The best result we can hope

to achieve is for the entries of X_δ to be very small. Thus, instead of aiming to show that X is extreme, we aim to show that X is close to being extreme in the sense that X_δ is small. We will call such points **extreme candidates**.

We can determine if a point X is an extreme candidate of $\mathcal{D}_A$ using a modified version of Proposition 2.6. As an example, suppose we are attempting to show that X is a Euclidean extreme candidate. As a reminder, a point $Y \in \mathcal{D}_A(n)$ is a Euclidean extreme point if and only if the only solution to the linear equation

$$\Lambda_A(\beta)K_{A,Y} = 0$$

in the unknown $\beta \in SM_n(\mathbb{R})^g$ is $\beta = 0$. Thus, the first step in determining if X is an extreme candidate is to compute the null space $K_{A,X}$ using some numerical method. The linear equation $\Lambda_A(\beta)K_{A,X} = 0$ has a matrix representation which we will denote $M_{A,X,Euc}\beta' = 0$. This equation has a nontrivial solution if and only if $M_{A,X,Euc}$ has a nontrivial null space. Thus, determining if X is a Euclidean extreme candidate of $\mathcal{D}_A$ can be reduced to determining if $M_{A,X,Euc}$ has a a singular value that we call zero. We use the algorithm below to determine if such a singular value exists. We also use the algorithm below to determine which right singular vectors are in the null space of $L_A(X)$.

Algorithm 4.3. *Let the matrix $M \in M_{n\times m}(\mathbb{R})$ with singular values (or eigenvalues if M is symmetric) $\lambda_1, \lambda_2, \ldots, \lambda_\ell$ where $\ell = \min(n, m)$ such that $|\lambda_i| > |\lambda_{i+1}|$. Let $\epsilon_m, \epsilon_g > 0$ be given (ϵ_m will be referred to as the magnitude tolerance and ϵ_g will be referred to as the gap tolerance throughout this paper). A singular value λ_i, for $i = 2, 3, \ldots, \ell$, is said to be the* **first numerical zero** *if all of the following are true*

(1) for all $j < i$, λ_j is not the first numerical zero
(2) $|\lambda_i| < \epsilon_m$
(3) $|\lambda_i/\lambda_{i-1}| < \epsilon_g$.

In other words, a singular value λ_i is the first numerical zero if it is the first singular value to be both smaller than the magnitude tolerance and have a sufficiently large gap between it and the previous singular value.

A singular value λ_i is called a **numerical zero** *if there exists some $1 < j < i$ such that λ_j is the first numerical zero.*

For all of our experiments, we take $\epsilon_m = \epsilon_g = 10^{-15}$ when determining if a point is extreme, and $\epsilon_m = \epsilon_g = 10^{-13}$ when computing the null space of $L_A(X)$. These choices were made after extensive experimentation.

4.1.2. *Null Space Purification.* The discussion in Section 4.1.1 demonstrate the importance of limiting the numerical when computing the null space of $L_A(X)$. Improving the numerical accuracy of $K_{A,X}$ can significantly improve the accuracy of the Arveson, Euclidean, and matrix extreme equations. One potential avenue for this is to slightly perturb the extreme candidate X so that the first numerical zero of $L_A(X)$ is small. The question then arises as to how to compute such a perturbation.

The following algorithm, which we call **Null Space Purification** is an algorithm that computes such a perturbation by solving a linear program. Linear programs can be solved quickly and to a high degree of accuracy which makes this method particularly effective.

Algorithm 4.4 (Null Space Purification)**.** *Let $\mathcal{D}_A$ be a bounded free spectrahedron and pick an extreme candidate X of $\mathcal{D}_A$. Let $K_{A,X}$ denote the null space of $L_A(X)$ which we compute using floating point arithmetic, and let $k_{A,X}$ be the dimension of $K_{A,X}$. We know that $k_{A,X} \geq 1$*

Now, fix some $\epsilon > 0$ and let $\eta_\epsilon \in \mathbb{R}$, $X_\epsilon \in SM_n(\mathbb{R})^g$ be the solution to the linear program

$$\begin{aligned} \eta_\epsilon, X_\epsilon := \quad & \underset{\eta\in\mathbb{R}\ Y\in SM_n(\mathbb{R})^g}{\text{Minimizer}} \quad \eta \\ \text{s.t.} \quad & \eta \geq 0 \\ & \max_{i=1,2,\ldots,dn} \left[K_{A,X}^T L_A(X+Y) K_{A,X}\right]_{ii} \leq \eta \\ & ||Y||_\infty \leq \epsilon \end{aligned} \tag{4.1}$$

where $||\cdot||_\infty : SM_n(\mathbb{R})^g \to \mathbb{R}$ is defined as $||X||_\infty = \max_{i,j,k} |X_{kij}|$ and X_{kij} is the i,j entry of the kth matrix in the tuple X.

The use of Algorithm 4.3 allows us to set a gap and magnitude tolerance when determining the null space of $L_A(X)$. This can be done by first numerically computing the eigendecomposition of $L_A(X) = V^T D V$, using Algorithm 4.3 to determine which eigenvalues of $L_A(X)$ are numerically zero, and then letting $K_{A,X}$ be the space spanned by the eigenvectors corresponding to the numerically zero eigenvalues. $K_{A,X}$ can be expressed as a matrix with floating point entries whose columns that the eigevectors of $L_A(X)$ corresponding to the numerically zero eigenvalues of $L_A(X)$.

Proposition 4.5. *If $\epsilon > 0$ and $\eta_\epsilon, X_\epsilon$ are as above, then $\widehat{X}_\epsilon = X + X_\epsilon$ has the following properties.*

(1) If $\lambda = ||L_A(X) K_{A,X}||_2$, then $\eta_\epsilon \leq \lambda$.
(2) If ϵ is sufficiently small, then $||L_A(\widehat{X}_\epsilon) K_{A,X}||_2 \leq \eta_\epsilon$.

(3) *If ϵ is sufficiently small, then $L_A(\widehat{X}_\epsilon) \succeq 0$ in the sense that the eigenvalues of $L_A(\widehat{X}_\epsilon)$ that are not numerically zero are positive.*

Proof. To show Item 1, we note that $\eta = \lambda$, $Y = 0$ is a feasible point for Equation (4.1).

Now let $\nu_1, \nu_2, \ldots, \nu_{dn}$ be the eigenvalues of $\Lambda_A(X_\epsilon)$, $\lambda_1, \lambda_2, \ldots, \lambda_{dn}$ be the eigenvalues of $L_A(X)$, and $\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_{dn}$ be the eigenvalues of $L_A(\hat{X}_\epsilon)$ with the convention that the eigenvalues are in decreasing order by magnitude. Let $\lambda_i = ||L_A(X)K_{A,X}||$ with gap tolerance δ. Item 2 holds if and only if $|\hat{\lambda}_i| < \delta|\hat{\lambda}_{i-1}|$. By comparison with the Frobenius norm, $|\nu_j| \leq (gdn||A||_\infty)\epsilon$ for all $j = 1, 2, \ldots, dn$. Moreover, by assumption $|\lambda_i| < \delta|\lambda_{i-1}|$, so $\mu := \delta|\lambda_{i-1}| - |\lambda_i| > 0$. Thus, if $\epsilon = \mu/(3gdn||A||_\infty)$,

$$\begin{aligned} |\hat{\lambda}_i| &\leq |\lambda_i| + |\nu_i| \\ &\leq |\lambda_i| + \frac{\mu}{3} \\ &< \delta|\lambda_{i-1}| - \frac{\mu}{3} \leq \delta|\hat{\lambda}_{i-1}|, \end{aligned}$$

which proves Item 2. If we take $\epsilon = \min(\mu/(3gdn||A||_\infty), |\lambda_{i-1}|/(gdn||A||_\infty))$ then Item 3 holds as the numerically nonzero eigenvalues of $L_A(\hat{X}_\epsilon)$ are $\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_{i-1}$, and for $1 \leq j \leq i-1$, $|\nu_j| \leq |\lambda_{i-1}|$, $\lambda_j > 0$, and

$$\hat{\lambda}_j > \lambda_j - |\nu_j| > \lambda_{i-1} - \lambda_{i-1} = 0.$$

Thus Item 3 holds. ■

In order to increase the numerical accuracy of the extreme point candidates that we generate using Algorithm 4.1, after each dilation step we perturb the dilated point using null space purification. As the goal of these experiments is to generate MnotA extreme points without much consideration for the actual points generated, this perturbation is acceptable. If there is particular importance to the initial boundary point, the algorithm can be modified to avoid perturbing the original point, instead only perturbing the columns and rows added in the dilation. The use of null space purification greatly decreases the rate of failure in our experiments, especially for $g = 2$.

4.2. **Data From Our Experiements: Guide to the Tables.** In our experiments, we consider three different parameters g, d, and n_0 where the defining tuple $A \in SM_d(\mathbb{R})^g$ and the initial point, discussed in Algorithm 4.1, $Y^0 \in SM_{n_0}(\mathbb{R})^g$. For every pair g and n_0, we generated 10,000 extreme point candidates using Algorithm 4.1. The defining tuples used were randomly generated irreducible tuples $A \in SM_d(\mathbb{R})^g$

where $d = g, g+1, g+2, g+3$. For each defining tuple, 25 points were generated; 100 defining tuples were generated for every value of d. Moreover, the generated spectrahedra were checked to ensure they were bounded.

Throughout Section 4, our experimental data will be presented in tables with the same format as in Table 1. Importantly, the tables describe the properties of the final points generated by the algorithm, not any intermediates. Thus, in the language of Algorithm 4.1, if $Y^0 \in \mathcal{D}_A(n_0)$ is the initial boundary point and $Y^k \in \mathcal{D}_A(n_0+k)$ is the final point, only Y^k and not Y^j for any $0 \leq j < k$ will be represented in the table. For each table, all of the generated points started at the same level n_0, and the n given in column 3 is the level that the points ended at after being dilated.

For any given g, d, and n,

(1) #Mat not Arv, #Euc, and #Arv columns give how many of the points where MnotA extreme, Euclidean extreme, or Arveson extreme point candidates respectively
(2) ArvCT,MatCT column gives the Arveson extreme equation and matrix extreme equation counts in that order
(3) $K_{A,X}$ columns count the number of points with kernel dimension $k_{A,X} = 1, 2, 3, 4, 5, > 5$ (second number is the dimension of the space of all $\beta \in M_{n\times 1}(\mathbb{R})$ such that $\ker L_A(Y^0) \subseteq \ker \Lambda_A(\beta^T)$)
(4) #Fail column counts the number of points which failed to dilate to a Euclidean extreme point

In one case, a point was determined to be a MnotA extreme point candidate, but the kernel dimension was uncertain. This case is marked with a $1*$.

A summary of our conclusions from the experiments can be found in Section 6

4.3. **Matrix extreme points of spectrahedra for $g = 2$.** We now narrow our focus to the case where $g = 2$. In this case, we conducted the experiment described above, generating 10,000 extreme point candidates for $d = 2, 3, 4, 5$. Extreme point candidate generation for $g = 2$ has a failure rate which is much higher ($\sim 0.7\%$) than any other value of g that we tested. This higher rate of failure is the result of a large number of failed dilation steps which results in the tests taking significantly longer.

A common theme throughout all of our experiments is that we only find examples of MnotA extreme point candidates when the matrix extreme equation count is strictly less than the Arveson extreme equation count. That is, we only find MnotA extreme point candidates when the minimum kernel size of $L_A(X)$ necessary to be matrix extreme is strictly less than the minimum kernel size necessary to be Arveson

extreme. We would expect this behavior if the matrix extreme and Arveson extreme equations were randomly generated, but they have structure.

We do, however, find parameter ranges where the matrix extreme equation count is strictly smaller than the Arveson extreme equation count, but no MnotA extreme point candidates were found. Stronger still, we find parameters, such as $g = 2$, $d = 3$, $n = 5$, where we find Euclidean extreme points with kernel dimensions sufficiently large to be called matrix extreme, yet none were determined to be matrix extreme candidates.

g = 2, Starting $n_0 = 3$, 10000 Points														
g	d	n	#Mat not Arv	#Euc	#Arv	ArvCT, MatCT	$K_{A,X}$ 1	2	3	4	5	>5	#Fail
2	2	3	0	0	0	3,3	0	0	0	0	0	0	0
		4	0	0	0	4,4	0	0	0	0	0	0	0
		5	0	2500	2500	5,5	0	0	0	0	2500;4	0	0
		6	0	0	0	6,6	0	0	0	0	0	0	0
		7	0	0	0	7,6	0	0	0	0	0	0	0
	3	3	0	0	0	2,2	4;3	0	0	0	0	0	4
		4	0	1773	1746	3,3	0	27;3	1746;3	0	0	0	0
		5	0	502	432	4,3	0	0	70;3	432;3	0	0	0
		6	0	221	221	4,4	0	0	0	83;3	138;3	0	0
		7	0	0	0	5,4	0	0	0	0	0	0	0
	4	3	0	6	0	2,2	6;2	0	0	0	0	0	0
		4	0	2494	2494	2,2	0	956;2	1537;2	0	0	0	0
		5	0	0	0	3,3	0	0	0	0	0	0	0
		6	0	0	0	3,3	0	0	0	0	0	0	0
		7	0	0	0	4,3	0	0	0	0	0	0	0
	5	3	0	519	0	2,2	519;1	0	0	0	0	0	0
		4	0	1981	1981	2,2	0	828;1	1153;1	0	0	0	0
		5	0	0	0	2,2	0	0	0	0	0	0	0
		6	0	0	0	3,3	0	0	0	0	0	0	0
		7	0	0	0	3,3	0	0	0	0	0	0	0

TABLE 1

g = 2, Starting $n_0 = 4$, 10000 Points													
g	d	n	#Mat not Arv	#Euc	#Arv	ArvCT, MatCT	$K_{A,X}$ 1	2	3	4	5	>5	#Fail
2	2	4	0	0	0	4,4	0	0	0	0	0	0	0
		5	0	0	0	5,5	0	0	0	0	0	0	0
		6	0	0	0	6,6	0	0	0	0	2;6	0	2
		7	0	2498	2498	7,6	0	0	0	0	0	2498	0
		8	0	0	0	8,7	0	0	0	0	0	0	0
	3	4	0	0	0	3,3	9;5	0	0	0	0	0	9
		5	0	178	0	4,3	0	14;5	178;5	0	0	0	14
		6	0	1988	1973	4,4	0	0	15;5	713;5	1260;5	0	0
		7	0	179	171	5,4	0	0	0	8;5	171;5	0	0
		8	35	132	97	6,5	0	0	0	0	35;5	97	0
	4	4	0	0	0	2,2	19;4	0	0	0	0	0	19
		5	0	1816	1786	3,3	0	30;4	1786;4	0	0	0	0
		6	0	665	665	3,3	0	0	291;4	374;4	0	0	0
		7	0	0	0	4,3	0	0	0	0	0	0	0
		8	0	0	0	4,4	0	0	0	0	0	0	0
	5	4	0	25	0	2,2	25;3	0	0	0	0	0	0
		5	0	2475	2475	2,2	0	727;3	1748;3	0	0	0	0
		6	0	0	0	3,3	0	0	0	0	0	0	0
		7	0	0	0	3,3	0	0	0	0	0	0	0
		8	0	0	0	4,3	0	0	0	0	0	0	0

TABLE 2

g = 2, Starting $n_0 = 5$, 10000 Points														
g	d	n	#Mat not Arv	#Euc	#Arv	ArvCT, MatCT	$K_{A,X}$ 1	2	3	4	5	>5	#Fail
2	2	5	0	0	0	5,5	0	0	0	0	0	0	0
		6	0	0	0	6,6	0	0	1;8	0	0	0	1
		7	0	0	0	7,6	0	0	0	0	0	0	0
		8	0	0	0	8,7	0	0	0	0	0	2	2
		9	0	2497	2497	9,8	0	0	0	0	0	2497	0
	3	5	0	0	0	4,3	18;7	0	0	0	0	0	18
		6	0	30	0	4,4	0	26;7	30;7	0	0	0	26
		7	0	1332	1293	5,4	0	0	36;7	39;7	1293;7	0	36
		8	384	929	529	6,5	0	0	0	16;7	384;7	529	0
		9	0	79	74	6,5	0	0	0	0	5;7	74	0
	4	5	0	0	0	3,3	19;6	0	0	0	0	0	19
		6	0	1744	1707	3,3	0	37;6	1707;6	0	0	0	0
		7	0	498	447	4,3	0	0	51;6	447;6	0	0	0
		8	0	239	239	4,4	0	0	0	119;6	120;6	0	0
		9	0	0	0	5,4	0	0	0	0	0	0	0
	5	5	0	0	0	2,2	59;5	0	0	0	0	0	59
		6	0	1823	1724	3,3	0	99;5	1724;5	0	0	0	0
		7	0	618	618	3,3	0	0	266;5	352;5	0	0	0
		8	0	0	0	4,3	0	0	0	0	0	0	0
		9	0	0	0	4,3	0	0	0	0	0	0	0

TABLE 3

4.4. **Matrix Extreme Points of Spectrahedra for $g = 3$.** We conducted the experiments analogous to those in Section 4.3 for defining tuples $A \in SM_d(\mathbb{R})^3$ and $d = 3, 4, 5, 6$. As in $g = 2$, for parameters where the matrix extreme equation count is equal to the Arveson extreme equation count, we do not find any MnotA extreme point candidates. Aside from this, there are some notable distinctions between the $g = 2$ and $g = 3$ cases.

Firstly, we can see that only four points failed to dilate to either Arveson or matrix extreme for $g = 3$ compared to 209 points for $g = 2$. Because of this, we can see that for a given g, d, and n, we usually find points with only one of two different kernel dimensions. The failed points in the $g = 2$ data made it difficult for this phenomenon to be seen.

Secondly, there is a much larger array of parameters at which we find MnotA extreme point candidates. With the exception of $g = 3$, $d = 4$, $n = 5$ (and higher

values of n which no points dilated to), for every g, d, and n where the matrix extreme equation count is strictly less than the Arveson extreme equation count we find MnotA extreme point candidates. The $d = 4$, $n = 5$ exception may be due to experimental design as all the points that started at $n_0 = 2$ and $n_0 = 3$ only needed one dilation step to reach Arveson or matrix extreme, and all the points that started at $n_0 = 4$ needed at least 3.

g = 3, Starting $n_0 = 2$, 10000 Points													
g	d	n	#Mat not Arv	#Euc	#Arv	ArvCT, MatCT	$K_{A,X}$ 1	2	3	4	5	>5	#Fail
3	3	2	0	0	0	2,2	0	0	0	0	0	0	0
		3	0	2500	2500	3,3	0	0	2500;3	0	0	0	0
		4	0	0	0	4,4	0	0	0	0	0	0	0
		5	0	0	0	5,4	0	0	0	0	0	0	0
		6	0	0	0	6,5	0	0	0	0	0	0	0
	4	2	0	0	0	2,2	0	0	0	0	0	0	0
		3	261	2500	2239	3,2	0	261;2	2239;2	0	0	0	0
		4	0	0	0	3,3	0	0	0	0	0	0	0
		5	0	0	0	4,3	0	0	0	0	0	0	0
		6	0	0	0	5,4	0	0	0	0	0	0	0
	5	2	0	119	0	2,2	119;1	0	0	0	0	0	0
		3	0	2381	2381	2,2	0	428;1	1953;1	0	0	0	0
		4	0	0	0	3,2	0	0	0	0	0	0	0
		5	0	0	0	3,3	0	0	0	0	0	0	0
		6	0	0	0	4,3	0	0	0	0	0	0	0
	6	2	0	2500	2500	1,1	2500;0	0	0	0	0	0	0
		3	0	0	0	2,2	0	0	0	0	0	0	0
		4	0	0	0	2,2	0	0	0	0	0	0	0
		5	0	0	0	3,2	0	0	0	0	0	0	0
		6	0	0	0	3,3	0	0	0	0	0	0	0

TABLE 4

g = 3, Starting $n_0 = 3$, 10000 Points														
g	d	n	#Mat not Arv	#Euc	#Arv	ArvCT, MatCT	$K_{A,X}$ 1	2	3	4	5	>5	#Fail
3	3	3	0	0	0	3,3	0	0	0	0	0	0	0
		4	0	1	0	4,4	0	0	1;6	0	0	0	0
		5	0	2499	2499	5,4	0	0	0	0	2499;6	0	0
		6	0	0	0	6,5	0	0	0	0	0	0	0
		7	0	0	0	7,6	0	0	0	0	0	0	0
	4	3	0	0	0	3,2	0	0	0	0	0	0	0
		4	0	2256	2256	3,3	0	0	2256;5	0	0	0	0
		5	0	187	187	4,3	0	0	0	187;5	0	0	0
		6	15	57	42	5,4	0	0	0	15;5	42;5	0	0
		7	0	0	0	6,4	0	0	0	0	0	0	0
	5	3	0	0	0	2,2	0	0	0	0	0	0	0
		4	398	2500	2102	3,2	0	397;4	2102;4	0	0	0	1*
		5	0	0	0	3,3	0	0	0	0	0	0	0
		6	0	0	0	4,3	0	0	0	0	0	0	0
		7	0	0	0	5,4	0	0	0	0	0	0	0
	6	3	0	0	0	2,2	0	0	0	0	0	0	0
		4	0	2500	2500	2,2	0	401;3	2099;3	0	0	0	0
		5	0	0	0	3,2	0	0	0	0	0	0	0
		6	0	0	0	3,3	0	0	0	0	0	0	0
		7	0	0	0	4,3	0	0	0	0	0	0	0

TABLE 5

g = 3, Starting $n_0 = 4$, 10000 Points														
g	d	n	#Mat not Free	#Euc	#Arv	ArvCT, MatCT	$K_{A,X}$ 1	2	3	4	5	>5	#Fail
3	3	4	0	0	0	4,4	0	0	0	0	0	0	0
		5	0	0	0	5,4	0	0	0	0	0	0	0
		6	0	8	0	6,5	0	0	0	0	8	0	0
		7	0	2492	2492	7,6	0	0	0	0	0	2492	0
		8	0	0	0	8,6	0	0	0	0	0	0	0
	4	4	0	0	0	3,3	0	0	0	0	0	0	0
		5	0	0	0	4,3	0	0	0	0	0	0	0
		6	284	2459	2175	5,4	0	0	0	284	2175	0	0
		7	34	34	0	6,4	0	0	0	0	34	0	0
		8	0	7	7	6,5	0	0	0	0	0	7	0
	5	4	0	0	0	3,2	0	0	0	0	0	0	0
		5	0	2165	2163	3,3	0	2	2163	0	0	0	0
		6	64	335	271	4,3	0	0	64	271	0	0	0
		7	0	0	0	5,4	0	0	0	0	0	0	0
		8	0	0	0	5,4	0	0	0	0	0	0	0
	6	4	0	0	0	2,2	3	0	0	0	0	0	3
		5	361	2497	2136	3,2	0	361	2136	0	0	0	0
		6	0	0	0	3,3	0	0	0	0	0	0	0
		7	0	0	0	4,3	0	0	0	0	0	0	0
		8	0	0	0	4,3	0	0	0	0	0	0	0

TABLE 6

4.5. **Matrix Extreme Points of Spectrahedra for $g = 4$.** We conducted the same experiment described in Section 4.3 for defining tuples $A \in SM_d(\mathbb{R})^4$ and $d = 4, 5, 6, 7$.

Similarly to the $g = 3$ case, we find that the only MnotA extreme points that we find occur when the Arveson extreme equation count is strictly larger than the matrix extreme equation count. Moreover, at a majority of parameters where we do find the matrix extreme equation count to be strictly smaller than the Arveson extreme equation count, we do find MnotA extremepoints.

g = 4, Starting $n_0 = 2$, 10000 Points													
g	d	n	#Mat not Arv	#Euc	#Arv	ArvCT, MatCT	$K_{A,X}$ 1	2	3	4	5	>5	#Fail
4	4	2	0	0	0	2,2	0	0	0	0	0	0	0
		3	0	2500	2500	3,3	0	0	2500;4	0	0	0	0
		4	0	0	0	4,4	0	0	0	0	0	0	0
		5	0	0	0	5,4	0	0	0	0	0	0	0
		6	0	0	0	6,5	0	0	0	0	0	0	0
	5	2	0	0	0	2,2	0	0	0	0	0	0	0
		3	98	2500	2402	3,2	0	98;3	2402;3	0	0	0	0
		4	0	0	0	4,3	0	0	0	0	0	0	0
		5	0	0	0	4,3	0	0	0	0	0	0	0
		6	0	0	0	5,4	0	0	0	0	0	0	0
	6	2	0	0	0	2,2	0	0	0	0	0	0	0
		3	0	2500	2500	2,2	0	179;2	2321;2	0	0	0	0
		4	0	0	0	3,3	0	0	0	0	0	0	0
		5	0	0	0	4,3	0	0	0	0	0	0	0
		6	0	0	0	4,3	0	0	0	0	0	0	0
	7	2	2500	2500	0	2,1	2500;1	0	0	0	0	0	0
		3	0	0	0	2,2	0	0	0	0	0	0	0
		4	0	0	0	3,2	0	0	0	0	0	0	0
		5	0	0	0	3,3	0	0	0	0	0	0	0
		6	0	0	0	4,3	0	0	0	0	0	0	0

TABLE 7

g = 4, Starting $n_0 = 3$, 10000 Points														
g	d	n	#Mat not Arv	#Euc	#Arv	ArvCT, MatCT	$K_{A,X}$ 1	2	3	4	5	>5	#Fail
4	4	3	0	0	0	3,3	0	0	0	0	0	0	0
		4	0	0	0	4,4	0	0	0	0	0	0	0
		5	0	2500	2500	5,4	0	0	0	0	2500;8	0	0
		6	0	0	0	6,5	0	0	0	0	0	0	0
		7	0	0	0	7,5	0	0	0	0	0	0	0
	5	3	0	0	0	3,2	0	0	0	0	0	0	0
		4	2424	2424	0	4,3	0	0	2424;7	0	0	0	0
		5	0	70	70	4,3	0	0	0	70;7	0	0	0
		6	1	6	5	5,4	0	0	0	1;7	5;7	0	0
		7	0	0	0	6,4	0	0	0	0	0	0	0
	6	3	0	0	0	2,2	0	0	0	0	0	0	0
		4	0	2380	2380	3,3	0	0	2380;6	0	0	0	0
		5	16	120	104	4,3	0	0	16;6	104;6	0	0	0
		6	0	0	0	4,3	0	0	0	0	0	0	0
		7	0	0	0	5,4	0	0	0	0	0	0	0
	7	3	0	0	0	2,2	0	0	0	0	0	0	0
		4	188	2500	2312	3,2	0	188;5	2311;5	0	0	0	0
		5	0	0	0	3,3	0	0	0	0	0	0	0
		6	0	0	0	4,3	0	0	0	0	0	0	0
		7	0	0	0	4,3	0	0	0	0	0	0	0

TABLE 8

4.6. **Summary of experimental findings.** Our experiments explored $g = 2, 3, 4$ with d ranging from $d = g$ to $d = g + 3$ with n varying but never exceeding 8. We primarily focused on these parameter ranges both as a way of supporting the process of constructing exact examples and because for larger values of g, the dilation steps take significantly longer to solve. From the data we can make a number of empirical observations.

(1) For $g = 2, 3, 4$, we do find values of d and n where there are MnotA extreme points.
(2) g **strictly greater than** d we do not find any MnotA extreme points for $g = d$. In this case, we see that for $g = 2, 3, 4$ all of the points generated at $d = g$ that dilated to Arveson extreme ended at the exact same level n. We do not see this phenomenon happening in general for $d > g$.
(3) **Strict count inequalities.** Assume $3 \leq g < d$. The only MnotA extreme points that we find occur when the Arveson extreme equation count is strictly larger than the matrix extreme equation count.[1]

    Conversely, in thirteen of twenty cases, if the matrix extreme equation count is less than the Arveson extreme equation count for some g, d, and n, for n not too large, then we find a MnotA extremepoint for that set of parameters. The cases are described below.

(4) (a) $g = 2$
        (i) $d = 3$, $n = 5$
        (ii) $d = 3$, $n = 7$
        (iii) $d = 3$, $n = 9$
        (iv) $d = 4$, $n = 7$
    (b) $g = 3$
        (i) $d = 4$, $n = 5$
        (ii) $d = 4$, $n = 7$ (only 7 points were found with $n = 7$, which is a very small sample. It is likely, considering the dimensions, that the only points that can reach this level for the given n_0 are Arveson extreme candidates)
    (c) $g = 4$
        (i) $d = 5$, $n = 5$ (only 70 points)

Aside from these main observations, the following are also of interest.

(1) MnotA extreme points are only observed at

[1]We would expect this behaviour if the equations were randomly generated; however, the systems have structure.

(a) $g = 2$
  (i) $d = 3$, $n = 8$.
(b) $g = 3$
  (i) $d = 4$, $n = 3$
  (ii) $d = 4$, $n = 6$
  (iii) $d = 4$, $n = 7$
  (iv) $d = 5$, $n = 4$
  (v) $d = 5$, $n = 4$
  (vi) $d = 5$, $n = 6$
  (vii) $d = 6$, $n = 5$
(c) $g = 4$
  (i) $d = 5$, $n = 3$
  (ii) $d = 5$, $n = 4$
  (iii) $d = 5$, $n = 6$
  (iv) $d = 6$, $n = 5$
  (v) $d = 7$, $n = 2$
  (vi) $d = 7$, $n = 4$

Beware we can not conclude that for larger g matrix extreme points are more plentiful. For small g, particularly $g = 2$, a larger percent of points fail to dilate as in Algorithm 4.1. This causes our experiments to run slower and produce fewer extreme points per fixed number of start points.

(2) In each of our experiments we produce a point at level n (over which we have no control except for the starting level). Bounds on n are:
  (a) for $g = 2$ the largest n we found was 8. Here, starting size was 5
  (b) for $g = 3$ the largest n we found was 8. Here, starting size was 4
  (c) for $g = 4$ the largest n we found was 6. Here, starting size was 3

5. Exact Arithmetic Point Generation

This section gives a method for producing provable examples of MnotA extreme points. In experiments it has been effective at producing lots of examples when $g = 3$, $d = 3$, and $n = 3$. (Beyond these parameters we have not explored the algorithm much.) Recall one such example is in Section 3.

5.1. **An algorithm for finding exact arithmetic extreme points.**

Algorithm 5.1. *Let $A \in SM_d(\{-1, 0, 1\})^g$ such that $\mathcal{D}_A$ is a bounded real free spectrahedron and fix $n \in \mathbb{N}$. Pick a $K \in \{-1, 0, 1\}^{dn}$ uniformly at random and solve the*

linear systems

$$L_A(X)K = 0$$
$$\Lambda_A(\beta^T)K = 0$$

for $X \in SM_n(\mathbb{Q})^g$ *and* $\beta \in M_{n\times 1}(\mathbb{Q})^g$.

(1) *If no solution exists for this* K*, choose a new* $K \in \{-1, 0, 1\}^{dn}$ *uniformly at random and solve the linear systems.*

(2) *If one solution exists for this* K*, we must then check that* $L_A(X)$ *is positive semidefinite. If* $L_A(X)$ *is not positive semidefinite, we discard this* K *and choose a new* $K \in \{-1, 0, 1\}^{dn}$ *uniformly at random and solve the linear systems.*

(3) *If there are infinitely many solutions, we then pick a tuple* X *in the solution space such that* $L_A(X)$ *is positive semidefinite.*

(4) *Once we have such an* X *and* β*, we let*

$$\hat{Y}(\hat{\alpha}) = \begin{pmatrix} X & \hat{\alpha}\beta \\ \hat{\alpha}\beta^T & 0 \end{pmatrix}$$

where $\hat{\alpha} \in \mathbb{R}$*. Let* α *denote the smallest non zero root of the derivative* $p_1(\hat{\alpha}) := \frac{d\chi_{\hat{\alpha}}(t)}{dt}_{|t=0}$ *of the characteristic polynomial* $\chi_{\hat{\alpha}}(t)$ *of* $L_A(\hat{Y}(\hat{\alpha}))$*.*

(5) *Denote* $p_2(\hat{\alpha}) := \frac{d^2\chi_{\hat{\alpha}}(t)}{d^2t}_{|t=0}$*. If* $p_2(\hat{\alpha}) = 0$*, then we generate a new* X *and* K *and repeat the process; if not then we conclude our search by setting*

$$Y := \hat{Y}(\alpha).$$

The algorithm uses exact arithmetic so that A*,* Y*, and* K *have entries which are algebraic numbers.*

Theorem 5.2. *If the above algorithm terminates, the generated point* Y *will belong to* $\mathcal{D}_A$ *and have* $k_{A,Y} \geq 2$*. Hence, if* $g = 3$*,* $d = 4$*, and* $Y \in SM_3(\mathbb{R})^3$*, we have that the Arveson Equation* (2.4) *has more unknowns than constraints, so implies* Y *is not an Arveson extreme point.*

Proof. Let X, β, K, and α be given by the algorithm above and let

$$Y = \begin{pmatrix} X & \alpha\beta \\ \alpha\beta^T & 0 \end{pmatrix}.$$

We know that

$$L_A(Y) = \Pi^T \begin{pmatrix} L_A(X) & \alpha\Lambda_A(\beta) \\ \alpha\Lambda_A(\beta^T) & I \end{pmatrix} \Pi$$

for some Π unitary (namely the canonical shuffle), so letting

$$K' = \Pi^T \begin{pmatrix} K \\ 0 \end{pmatrix},$$

we see that $L_A(Y)K' = 0$ as

$$\begin{aligned} L_A(Y) &= \Pi^T \begin{pmatrix} L_A(X) & \alpha\Lambda_A(\beta) \\ \alpha\Lambda_A(\beta^T) & I \end{pmatrix} \Pi K' \\ &= \Pi^T \begin{pmatrix} L_A(X)K & 0 \\ \alpha\Lambda_A(\beta^T)K & 0 \end{pmatrix} = 0 \end{aligned}$$

as $L_A(X)K = \Lambda_A(\beta^T)K = 0$. Thus, the characteristic polynomial $\chi_\alpha(t)$ of $L_A(Y)$ has no constant term. Moreover, by the definition of α, we have $\chi'_\alpha(0) = 0$ and $\chi''_\alpha(0) \neq 0$. Thus $\chi_\alpha(t) = t^2 q_\alpha(t)$ for some polynomial q_α such that $q_\alpha(0) \neq 0$, consequently $L_A(Y)$ has a null space of dimension 2.

We now aim to show that $Y \in \mathcal{D}_A$. To do this, we first note that taking $\hat{\alpha} = 0$, we get that $L_A(\hat{Y}(0))$ is unitarily equivalent to

$$\begin{pmatrix} L_A(X) & 0 \\ 0 & I \end{pmatrix}$$

which is clearly positive semidefinite. Moreover, since for all $\hat{\alpha}$, a $L_A(\hat{Y}(\hat{\alpha}))K' = 0$, we have $\chi_{\hat{\alpha}}(t) = t(t - \lambda_2(\hat{\alpha})) \cdots (t - \lambda_{nd+d}(\hat{\alpha}))$ where the $\lambda_i(\hat{\alpha})$ are the eigenvalues of $L_A(\hat{Y}(\hat{\alpha}))$. Thus, $p_1(\hat{\alpha}) = (-1)^{(n+1)d-1}\lambda_2(\hat{\alpha}) \cdots \lambda_{nd+d}(\hat{\alpha})$. We note that $p_1(\hat{\alpha}) = 0$ if and only if $\lambda_i(\hat{\alpha}) = 0$ for some $i = 2, 3, \ldots, nd + d$ and we pick α so that it is the smallest positive root of $p_1(\hat{\alpha})$. Thus, there must be some i such that $\lambda_i(\alpha) = 0$. Moreover, if $\lambda_j(\alpha) < 0$, then, by the intermediate value theorem since $\lambda_j(0) > 0$, there must exist some $0 < \alpha_0 < \alpha$ where $\lambda_j(\alpha_0) = 0$. This implies $p_1(\alpha_0) = 0$, a contradiction to the assumption that α is the smallest positive root. Thus for $j \neq i$, $\lambda_j(\alpha) \geq 0$ and hence $Y \in \mathcal{D}_A$.

The Arveson equation count (2.8) for $g = 3$, $d = 4$, and $n = 3$ is 3. So by Corollary 2.7 if $Y \in \mathcal{D}_A(3)$ then $k_{A,Y} = 2 < 3$ implies that Y is not Arveson extreme. ■

Thus, any point produced with this algorithm at these parameters cannot be Arveson extreme, but is potentially matrix extreme. The matrix $L_A(Y)$ will have entries that are algebraic numbers, and so the kernel and matrix extreme equations can, in principle, be computed in exact arithmetic.

5.2. **A property of χ_α.**

Lemma 5.3. *If*

$$Y = \begin{pmatrix} X & \alpha\beta \\ \alpha\beta^T & 0 \end{pmatrix}$$

for $X \in SM_n(\mathbb{R})^g$, $\beta \in M_{n\times 1}$, and $\alpha \in \mathbb{R}$, then the characteristic polynomial $\chi_\alpha(t)$ of $L_A(Y)$ has coefficients that are degree dn polynomials in α^2.

Proof. Using the canonical shuffle, we can show that $L_A(Y)$ is unitarily equivalent to

$$Z = \begin{pmatrix} L_A(X) & \alpha\Lambda_A(\beta) \\ \alpha\Lambda_A(\beta^T) & I \end{pmatrix}.$$

The eigenvalues of a matrix, and thus the characteristic polynomial, are invariant under unitary equivalence, so it is sufficient to compute the characteristic polynomial of Z. Note that $Z \in SM_{d(n+1)}(\mathbb{R}[\alpha])$ and thus $\chi_\alpha(t) \in \mathbb{R}[\alpha][t]$.

$$\chi_\alpha(t) = \det \begin{pmatrix} L_A(X) - tI & \alpha\Lambda_A(\beta) \\ \alpha\Lambda_A(\beta^T) & (1-t)I \end{pmatrix}$$

so for $t \neq 1$, we can use the Schur determinant formula to show that

$$\begin{aligned} \det \begin{pmatrix} L_A(X) - tI & \alpha\Lambda_A(\beta) \\ \alpha\Lambda_A(\beta^T) & (1-t)I \end{pmatrix} &= \det((1-t)I) \det(L_A(X) - tI - \frac{\alpha^2}{(1-t)}\Lambda_A(\beta)\Lambda_A(\beta^T)) \\ &= (1-t)^d \det(L_A(X) - tI - \frac{\alpha^2}{(1-t)}\Lambda_A(\beta)\Lambda_A(\beta^T)). \end{aligned}$$

Thus $\chi_\alpha(t)$ depends only on α^2 for $t \neq 1$. ■

5.2.1. *Experiments with method of fixed kernel.* We ran the procedure one hundred times; every time an X, β, and K were found. Each time the procedure was run, multiple kernels K were generated until an X and β could be found such that $L_A(X)K = 0$ and $\Lambda_A(\beta^T)K = 0$. We have only run this method for a single fixed A.

On two randomly chosen occasions, we went through the hour long process of trying to compute the matrix extreme equations exactly. While the equations could in princple be computed in exact arithmetic, the calculation for determining if the matrix extreme equations had a null space became too difficult to solve.

We then numerically determined the singular values of the matrix extreme equations, Equation (2.6). In every case, the largest singular value was less than 4 and 80 of the points had smallest singular value on the order of 10^{-4}. Hence, we are confident that those 80 points are matrix extreme. In order to be Arveson extreme, the points would require a kernel dimension of at least 3. However, in all cases, we computed the eigenvalues of $L_A(X)$ numerically determined two of the eigenvalues to be zero. This determination was made as the smallest two eigenvalues were on the order of 10^{-15} in all cases, and the next smallest eigenvalue was on the order of 10^0. Thus, the points could have a kernel of at most dimension 2.

Remark 5.4. *Nowhere in Theorem 5.2 do we use the fact that K was chosen from $\{-1, 0, 1\}$. In fact, we may pick $K \in \mathbb{Q}^{dn}$. The kernel K was picked in this manner to reduce the computational complexity of the problem.*

6. Conclusions

We have algorithms which reliably produced MnotA extreme points when $g = 3$. In addition when $g = 4$ we have produced "by hand" a MnotA extreme point.

We have "perfected" a numerical algorithm for producing MnotA extreme candidates as described in Section 4.1. The reliability of this algorithm relies on a new technique we call null space purification. This modified algorithm has a much lower rate of failure to the unmodified algorithm used previously [EH19], especially in the $g = 2$ case. The null space purification algorithm yields extreme point candidates with numerical accuracy on the order of 10^{-13} as opposed to the 10^{-7} accuracy that we find using semidefinite programming alone which allows us to use tighter tolerances when determining if a point is an extreme candidate.

The experiments described in Section 4 yield the following interesting results. Firstly and most importantly, for $g = 2, 3, 4$ we find MnotA extreme candidates. Secondly, we never find any MnotA extreme candidates when $g = d$. Thirdly, we only find MnotA extreme candidates when the Arveson extreme equation count is strictly greater than the matrix extreme equation count. Conversely, for $g = 3, 4$ and $d > g$, in thirteen of sixteen cases, when the Arveson extreme equation count $\left\lceil \frac{gn}{d} \right\rceil$ is larger than the matrix extreme equation count $\left\lceil \frac{gn(n+1)-2}{2dn} \right\rceil$, we find MnotA extreme candidates. The three exceptions are potentially explainable through experimental design. We speculate that for $g = 3, 4$ and $d > 4$, if the Arveson extreme count is strictly greater than the matrix extreme equation count, then there is a MnotA extreme for that value of g, d, n.

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Appendix Contributions of Aidan Epperly

Eric Evert, a Ph.D. student of mine and now a postdoc, began some experiments on optimizing linear functionals over free spectrahedra (the solution set of a free linear matrix inequality). Of course the maximizer is an extreme point. However, for free spectrahedra there are three natural types of extreme points:

ordinary Euclidean extreme $\supset$ matrix extreme $\supset$ free extreme .

Extensive experiments show that: Fixing a dimension of a free spectrahedron and randomly generating a linear functional yields a maximizer which is very likely free extreme. (When Epperly became involved he read this paper and understood it quickly with almost no help.) One never even sees serious evidence that a matrix extreme point exists, hence there was the possibility that they do not exist for free spectrahedra. This has been an open question for a few years or longer depending on how one counts.

Alas matrix extreme points do exist which is the subject of this work. It started when Evert found an exact arithmetic formula for the example given here when $g = 4$. This is remarkable in that it involves exact eigenvalue/vectors for 15×15 matrices. Validating the example required converting a theorem of Kriel to an algorithm which Evert , Klep and Epperly did and perfected.

Epperly is outstanding at scientific computation; he has made serious contributions to Evert's extreme point package. First he found an inefficiency with the code that reduced its numerical precision. Also he greatly improved passing of information inside the code, so now we can see more aspects of extreme points. The next release of the package will be seriously influenced by Epperly.

Now to the case of $g = 2, 3$. Epperly set up algorithms and experiments and he produced the data and conclusions of Chapter 4. Here a big tool where Epperly did much of the development was 'null space purification'. This taking precision from 10^{-7} to 10^{-12} was critical to finding many candidates for matrix but not free extreme points. In the course of this he found numerical example spectrahedra with very simple coefficient matrices (all 0, 1, -1 entries).

Section 5 gave an exact arithmetic approach Klep developed which, when applied to Epperly's simple numerical examples above, gave many $g = 3$ exact examples.

I would also add that Epperly, being an articulate fellow, did much more of the actual writing of the paper than is usual in the honors theses I have directed.

J. William Helton