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Geometry of the copositive and completely positive cones

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ABSTRACT

The copositive cone, and its dual the completely positive cone, have useful applications in optimisation, however telling if a general matrix is in the copositive cone is a co-NP-complete problem. In this paper we analyse some of the geometry of these cones. We discuss a way of representing all the maximal faces of the copositive cone along with a simple equation for the dimension of each one. In doing this we show that the copositive cone has faces which are isomorphic to positive semidefinite cones. We also look at some maximal faces of the completely positive cone and find their dimensions. Additionally we consider extreme rays of the copositive and completely positive cones and show that every extreme ray of the completely positive cone is also an exposed ray, but the copositive cone has extreme rays which are not exposed rays.

1. Introduction

The copositive and completely positive cones are proper cones (i.e. closed, convex, pointed and full dimensional), which are the duals of each other [1, p. 71]. Surveys on copositivity and complete positivity are provided by [2,3].

The copositive and completely positive cones, denoted $\mathcal{C}$ and $\mathcal{C}^*$ respectively, are of interest due to their applications in optimisation, especially in creating convex formulations of NP-hard problems. It has been shown in [4] that if we consider the quadratic binary problem, where the symmetric matrix Q and the vectors $c, a_1, \dots, a_m$ are of order n, the vector b is of order m and $B \subseteq \{1, \dots, n\}$,

$$\begin{aligned} \min\quad & x^{\mathsf T} Q x + 2c^{\mathsf T} x, \\ \text{s.t.}\quad & a_i^{\mathsf T} x = b_i \quad (i = 1, \dots, m), \\ & x \geqslant 0, \\ & x_j \in \{0, 1\} \quad (j \in B), \end{aligned}$$

then this can be reformulated under mild assumptions into the following completely positive problem which is a convex linear problem,

$$\begin{aligned} \min\quad & \langle Q, X\rangle + 2c^{\mathsf T} x, \\ \text{s.t.}\quad & a_i^{\mathsf T} x = b_i \quad (i = 1, \dots, m), \\ & \langle a_i a_i^{\mathsf T}, X\rangle = b_i^2 \quad (i = 1, \dots, m), \\ & (x)_j = (X)_{jj} \quad (j \in B), \\ & \begin{pmatrix} 1 & x^{\mathsf T} \\ x & X \end{pmatrix} \in \mathcal{C}^*. \end{aligned}$$

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An example of an NP-hard problem which can be formulated like this is the maximum clique problem [5,6]. If we let $\omega(G)$ be the clique number of a graph G with adjacency matrix A_G and let e be the all-ones vector, then

$$\frac{1}{\omega(G)} = \min\left\{x^\mathsf{T}\left(ee^\mathsf{T} - A_G\right)x \;\middle|\; e^\mathsf{T}x = 1,\ x \geqslant 0\right\}.$$

The use of the copositive cone in the formulations comes from the standard Lagrangian approach which means that if we consider a proper cone $\mathcal{K}$ and its dual $\mathcal{K}^*$ then

$$\begin{aligned} \min \quad & \langle Q, X\rangle, \\ \text{s.t.} \quad & \langle A_i, X\rangle = b_i \quad (i = 1, \ldots, m), \\ & X \in \mathcal{K}, \end{aligned}$$

is, under some regularity conditions (e.g. Slater's Condition), equivalent to

$$\begin{aligned} \max \quad & \sum_{i=1}^{m} b_i y_i, \\ \text{s.t.} \quad & Q - \sum_{i=1}^{m} y_i A_i \in \mathcal{K}^*, \\ & y_i \in \mathbb{R} \quad (i = 1, \ldots, m). \end{aligned}$$

In this paper we will be looking specifically at the geometry of the copositive and completely positive cones. This includes studying extreme and exposed rays of both cones, as well as maximal faces of them. Every point on the boundary of a proper cone is a member of a maximal face so the union of the maximal faces is equal to the boundary of the cone.

We will start in Section 2 by considering relationships between a general proper cone and its dual in terms of their rays and exposed faces. Some of these results will then be demonstrated using the copositive and completely positive cones in Section 3. After this, in Section 4, we will show that every extreme ray of the completely positive cone is also an exposed ray, which is in contrast to the copositive cone which we will show to have extreme rays which are not exposed. We also present here some exposed rays of the copositive cone. In Section 5 we will use results developed in this paper in order to find the form of the maximal faces of the copositive cone and their dimensions. In doing this we will also find faces of the copositive cone which are isomorphic to positive semidefinite cones. In Sections 6 and 7 we finish by looking at some of the maximal faces of the completely positive cone.

We will be using the following notation in this paper:

$$\begin{aligned} &\text{Inner product for symmetric matrices, } \langle A, B\rangle := \operatorname{trace}(AB), \\ &\text{Nonnegative orthant, } \mathbb{R}^n_+ := \left\{x \in \mathbb{R}^n \;\middle|\; x \geqslant 0\right\}, \\ &\text{Strictly positive orthant, } \mathbb{R}^n_{++} := \left\{x \in \mathbb{R}^n \;\middle|\; x > 0\right\}, \\ &\text{Set of symmetric matrices, } \mathcal{S}^n := \left\{A \in \mathbb{R}^{n\times n} \;\middle|\; A = A^\mathsf{T}\right\}, \\ &\text{Set of nonnegative symmetric matrices, } \mathcal{N}^n := \left\{A \in \mathcal{S}^n \;\middle|\; A \geqslant 0\right\}, \\ &\text{Positive semidefinite cone, } \mathcal{S}^n_+ := \left\{A \in \mathcal{S}^n \;\middle|\; x^\mathsf{T}Ax \geqslant 0 \text{ for all } x \in \mathbb{R}^n\right\} \\ &\qquad\qquad = \left\{\sum_i a_i a_i^\mathsf{T} \;\middle|\; a_i \in \mathbb{R}^n \text{ for all } i\right\}, \\ &\text{Copositive cone, } \mathcal{C}^n := \left\{A \in \mathcal{S}^n \;\middle|\; x^\mathsf{T}Ax \geqslant 0 \text{ for all } x \in \mathbb{R}^n_+\right\}, \\ &\text{Completely positive cone, } \mathcal{C}^{*n} := \left\{\sum_i a_i a_i^\mathsf{T} \;\middle|\; a_i \in \mathbb{R}^n_+ \text{ for all } i\right\}. \end{aligned}$$

For the matrix sets we will usually omit n when the dimension is apparent from the context.

For a closed convex set $\mathcal{L}$ we shall use $\operatorname{bd}(\mathcal{L})$ to denote its boundary, $\operatorname{int}(\mathcal{L})$ to denote its interior and $\operatorname{reint}(\mathcal{L})$ to denote its relative interior.

The last bit of notation that we will mention for the moment is e_i as the unit vector with the ith entry equal to one and all other entries equal to zero.

One thing to note from the definitions is it can be immediately seen that

$$\mathcal{C}^* \subseteq (\mathcal{S}_+ \cap \mathcal{N}) \subseteq (\mathcal{S}_+ + \mathcal{N}) \subseteq \mathcal{C}.$$

We finish our introduction with some properties of copositive matrices.

Theorem 1.1. *Let A be a copositive matrix, then we have that*:

(i) *Every principal submatrix of A must also be copositive (where a principal submatrix of A is a matrix formed by deleting any rows along with the corresponding columns from A).*
(ii) $(A)_{ii} \geqslant 0$ *for all i.*
(iii) $(A)_{ij} \geqslant -\sqrt{(A)_{ii}(A)_{jj}}$ *for all i, j.*
(iv) *If $(A)_{ii} = 0$, then $(A)_{ij} \geqslant 0$ for all j.*
(v) *If P is a permutation matrix and D is a nonnegative diagonal matrix, then $PDADP^{\mathsf{T}} \in \mathcal{C}$.*
(vi) *If there exists a strictly positive vector v such that $v^{\mathsf{T}}Av = 0$, then $A \in \mathcal{S}_+$.*

Proof. A proof for (i)–(iv) can be found in [7], (v) comes trivially from the fact that $DP^{\mathsf{T}}\mathbb{R}^n_+ \subseteq \mathbb{R}^n_+$, and (vi) comes directly from [8, Lemma 1]. □

2. Geometry of general proper cones

We start by analysing the relationships between the extreme rays in a general proper cone and the maximal faces in its dual. In order to do this we first need some definitions. The definitions for a face, an exposed face, an exposed ray and an extreme ray are equivalent to those used in [9, Section 18].

Definition 2.1. A face of a closed convex set $\mathcal{L} \subseteq \mathbb{R}^n$ is a convex subset $\mathcal{F}$ of $\mathcal{L}$ such that every closed line segment in $\mathcal{L}$ with a relative interior point in $\mathcal{F}$ must have both end points in $\mathcal{F}$. A facet of a closed convex set $\mathcal{L}$ is a face of the set with dimension equal to $\dim \mathcal{L} - 1$. An extreme point of a closed convex set $\mathcal{L}$ is a face of the set with dimension equal to zero.

Definition 2.2. Let $\mathcal{L}$ be a closed convex set in $\mathbb{R}^n$ and $\emptyset \neq \mathcal{F} \subseteq \mathcal{L}$. $\mathcal{F}$ is an exposed face of $\mathcal{L}$ if it is the intersection of $\mathcal{L}$ and a non-trivial supporting hyperplane, i.e. if there exists $a \in \mathbb{R}^n \setminus \{0\}$, $b \in \mathbb{R}$ such that $\mathcal{L} \subseteq \{x \in \mathbb{R}^n \mid \langle x, a\rangle \geqslant b\}$ and $\mathcal{F} = \{x \in \mathcal{L} \mid \langle x, a\rangle = b\}$. An exposed point of a closed convex set $\mathcal{L}$ is an exposed face of the set with dimension equal to zero. (Rockafellar also refers to $\mathcal{L}$ and $\emptyset$ as exposed faces, however we shall exclude these. In much of the literature, for example [10], these faces are called improper exposed faces whilst the exposed faces that we will be considering are called (proper) exposed faces.)

Remark 2.3. Every exposed face must also be a face.

Theorem 2.4. *Every face of a full dimensional closed convex set $\mathcal{L}$ which is not equal to $\mathcal{L}$ is contained within an exposed face.*

Proof. If $\mathcal{F}_1 \neq \mathcal{L}$ is an arbitrary face of $\mathcal{L}$, then we must have $\mathcal{F}_1 \subseteq \mathrm{bd}(\mathcal{L})$. Let x be in the relative interior of $\mathcal{F}_1$. By the supporting hyperplane theorem there exists an exposed face $\mathcal{F}_2$ such that $x \in \mathcal{F}_2$. Therefore $\mathcal{F}_2 \cap \mathrm{reint}(\mathcal{F}_1) \neq \emptyset$ so from [9, Theorem 18.1] we must have $\mathcal{F}_1 \subseteq \mathcal{F}_2$. □

Definition 2.5. A face $\mathcal{F}_1$ is a maximal face of a full dimensional closed convex set $\mathcal{L}$ if $\mathcal{F}_1 \neq \mathcal{L}$ and there does not exist a face $\mathcal{F}_2 \neq \mathcal{L}$ such that $\mathcal{F}_1 \subset \mathcal{F}_2$.

Remark 2.6. From Theorem 2.4 it can be immediately seen that every maximal face must also be an exposed face.

Remark 2.7. The maximal faces of a polyhedron are its facets and the maximal faces of an n-sphere are the points on its boundary.

The following theorem contributes towards our motivation for looking at the set of maximal faces as it means that the hyperplanes giving maximal faces are desirable in a cutting plane algorithm.

Theorem 2.8. *Let $\mathbb{M}$ be the set of maximal faces of a full dimensional closed convex set $\mathcal{L}$, and let $\mathbb{S}$ be an arbitrary set of its faces, none of which are equal to the complete set. Then,*

$$\bigcup_{\mathcal{F}\in\mathbb{S}} \mathcal{F} = \mathrm{bd}(\mathcal{L}) \quad \Leftrightarrow \quad \mathbb{M} \subseteq \mathbb{S}.$$

Proof. ($\Leftarrow$) By the supporting hyperplane theorem, every point on the boundary of $\mathcal{L}$ must be a member of an exposed face and therefore must also be a member of a maximal face. This implies that $\mathrm{bd}(\mathcal{L}) = \bigcup_{\mathcal{F}\in\mathbb{M}} \mathcal{F}$.

($\Rightarrow$) Suppose by contradiction that $\bigcup_{\mathcal{F}\in\mathbb{S}} \mathcal{F} = \mathrm{bd}(\mathcal{L})$ and there exists a maximal face $\mathcal{F}_1 \notin \mathbb{S}$. We now consider an arbitrary point $x \in \mathrm{reint}(\mathcal{F}_1)$. We must have that $x \in \mathrm{bd}(\mathcal{L})$, therefore there exists a face $\mathcal{F}_2 \in \mathbb{S}$ such that $x \in \mathcal{F}_2$. This implies that $\mathcal{F}_2 \cap \operatorname{reint}(\mathcal{F}_1) \neq \emptyset$ and so from [9, Theorem 18.1] we get that $\mathcal{F}_1 \subset \mathcal{F}_2$, implying that $\mathcal{F}_1$ cannot be a maximal face. □

We now switch our focus to rays, in particular the exposed and extreme rays. If we consider an arbitrary $x \in \mathbb{R}^n \setminus \{0\}$, then the ray given by x is defined to be the set $\{\alpha x \mid \alpha \geqslant 0\}$.

Definition 2.9. $x \in \mathcal{K} \setminus \{0\}$ gives an exposed ray of a proper cone $\mathcal{K}$ if there exists an exposed face $\mathcal{F}$ of $\mathcal{K}$ such that

$$\mathcal{F} = \{\alpha x \mid \alpha \geqslant 0\}.$$

We write $\operatorname{Exp}(\mathcal{K})$ for the set of elements giving exposed rays of the cone $\mathcal{K}$.

Definition 2.10. $x \in \mathcal{K} \setminus \{0\}$ gives an extreme ray of a proper cone $\mathcal{K}$ if

$$y, z \in \mathcal{K}, \quad y + z = x \quad \Rightarrow \quad y, z \in \{\alpha x \mid \alpha \geqslant 0\}.$$

We write $\operatorname{Ext}(\mathcal{K})$ for the set of elements giving extreme rays of the cone $\mathcal{K}$.

Theorem 2.11 *(Straszewicz's Theorem). (See [9, Theorem 18.6].) For a closed convex set, the set of exposed points is a dense subset of the set of extreme points.*

This can be extended to rays of a proper cone, giving the following.

Theorem 2.12. *For a proper cone $\mathcal{K}$,*

$$\operatorname{Exp}(\mathcal{K}) \subseteq \operatorname{Ext}(\mathcal{K}) \subseteq \operatorname{cl}\bigl(\operatorname{Exp}(\mathcal{K})\bigr).$$

Proof. As $\mathcal{K}$ is a closed pointed cone there exists a bounded base of it, $\mathcal{B} = \mathcal{H} \cap \mathcal{K}$, for some hyperplane $\mathcal{H}$. We have that $x \in \operatorname{Ext}(\mathcal{K})$ ($x \in \operatorname{Exp}(\mathcal{K})$) if and only if there exists $\alpha > 0$ such that αx is an extreme (exposed) point of $\mathcal{B}$. We now consider Straszewicz's Theorem to get the desired result. □

The final definition we give in this section is that of the dual of a set.

Definition 2.13. For a set $\mathcal{K} \subseteq \mathbb{R}^n$, the dual cone is defined as

$$\mathcal{K}^* := \bigl\{a \in \mathbb{R}^n \bigm| \langle a, x\rangle \geqslant 0 \text{ for all } x \in \mathcal{K}\bigr\}.$$

Theorem 2.14. *(See [1, Chapter 1].) If $\mathcal{K}$ is a proper cone then so is its dual $\mathcal{K}^*$ and we have that $\mathcal{K}^{**} = \mathcal{K}$.*

We will now consider how the faces of one proper cone are related to points in its dual.

Theorem 2.15. *$\mathcal{F}$ is an exposed face of a proper cone $\mathcal{K}$ if and only if there exists an $a \in \mathcal{K}^* \setminus \{0\}$ such that*

$$\mathcal{F} = \mathcal{F}(\mathcal{K}, a) := \bigl\{x \in \mathcal{K} \bigm| \langle x, a\rangle = 0\bigr\}.$$

Proof. From [11, p. 51] we have that

$y \in \mathcal{K}^*$ if and only if $-y$ is the normal of a hyperplane that supports $\mathcal{K}$ at the origin.

If we now consider any nonzero point in a face of $\mathcal{K}$, then from the definition of a face we get that the ray given by this point must also be contained within the face. This implies that all nonempty faces of a proper cone contain the origin.

Combining these two facts gives us the required result. □

Using the following observation we now get a similar result relating the maximal faces of one proper cone to the extreme rays in its dual. This lemma can be immediately seen from the definition of $\mathcal{F}(\mathcal{K}, a)$ in Theorem 2.15 and the definition of the dual, so it is presented without proof.

Lemma 2.16. *For $\{a_1, \dots, a_m\} \subset \mathcal{K}^*$, we have that*

$$\mathcal{F}\left(\mathcal{K}, \sum_{i=1}^{m} a_i\right) = \bigcap_{i=1}^{m} \mathcal{F}(\mathcal{K}, a_i),$$

where we extend the definition of $\mathcal{F}(\mathcal{K}, a)$ such that $\mathcal{F}(\mathcal{K}, 0) := \mathcal{K}$.

Theorem 2.17. *If $\mathcal{F}$ is a maximal face of a proper cone $\mathcal{K}$ then there exists an $a \in \operatorname{Ext}(\mathcal{K}^*)$ such that*

$$\mathcal{F} = \mathcal{F}(\mathcal{K}, a).$$

Proof. Let $\mathcal{F}$ be a maximal face of $\mathcal{K}$. Then $\mathcal{F}$ is an exposed face, and so by Theorem 2.15 we have $\mathcal{F} = \mathcal{F}(\mathcal{K}, a)$ for some $a \in \mathcal{K}^* \setminus \{0\}$. It is a well-known result that a can be decomposed as $a = \sum_{j \in \mathcal{J}} a_j$, where $\{a_j\}_{j \in \mathcal{J}} \subseteq \operatorname{Ext}(\mathcal{K}^*)$. This is in fact an extension of the Krein–Milman theorem [12]. Therefore

$$\begin{aligned}
\mathcal{F} = \mathcal{F}(\mathcal{K}, a) &= \mathcal{F}\left(\mathcal{K}, \sum_{j \in \mathcal{J}} a_j\right) \\
&= \bigcap_{j \in \mathcal{J}} \mathcal{F}(\mathcal{K}, a_j) \quad \text{(Lemma 2.16)} \\
&\subseteq \mathcal{F}(\mathcal{K}, a_j) \quad \text{for all } j \in \mathcal{J}.
\end{aligned}$$

For an arbitrary $j \in \mathcal{J}$ we have that $\mathcal{F}(\mathcal{K}, a_j)$ is an exposed face of $\mathcal{K}$ and because $\mathcal{F}$ is a maximal face we must have that $\mathcal{F} = \mathcal{F}(\mathcal{K}, a_j)$, completing the proof. □

The converse is not true as if $a \in \operatorname{Ext}(\mathcal{K}^*)$ then $\mathcal{F}(\mathcal{K}, a)$ is not necessarily a maximal face. We do however always get maximal faces from the exposed rays. Before we prove this we first need the following two trivial lemmas.

Lemma 2.18. *For $a \in \mathcal{K}^*$ and $x \in \mathcal{K}$,*

$$a \in \mathcal{F}(\mathcal{K}^*, x) \quad \Leftrightarrow \quad \langle a, x \rangle = 0 \quad \Leftrightarrow \quad x \in \mathcal{F}(\mathcal{K}, a).$$

Lemma 2.19. *For $a \in \mathcal{K}^*$, $\lambda > 0$, we have that*

$$\mathcal{F}(\mathcal{K}, \lambda a) = \mathcal{F}(\mathcal{K}, a).$$

Theorem 2.20. *If $\mathcal{K}$ is a proper cone and $a \in \operatorname{Exp}(\mathcal{K}^*)$, then $\mathcal{F}(\mathcal{K}, a)$ is a maximal face of $\mathcal{K}$.*

Proof. Consider an arbitrary $a \in \operatorname{Exp}(\mathcal{K}^*)$.

By the definition of an exposed ray and Theorem 2.15, there must exist $x \in \mathcal{K}$ such that $\mathcal{F}(\mathcal{K}^*, x) = \{\alpha a \mid \alpha \geqslant 0\}$.

From Lemma 2.18 this means that $x \in \mathcal{F}(\mathcal{K}, a)$ and for all $b \in \mathcal{K}^* \setminus \{\alpha a \mid \alpha \geqslant 0\}$, we have that $x \notin \mathcal{F}(\mathcal{K}, b)$.

From Lemma 2.19 we have that if $b = \alpha a$ where $\alpha > 0$, then $\mathcal{F}(\mathcal{K}, a) = \mathcal{F}(\mathcal{K}, b)$.

Therefore there does not exist $b \in \mathcal{K}^* \setminus \{0\}$ such that $\mathcal{F}(\mathcal{K}, a) \subset \mathcal{F}(\mathcal{K}, b)$.

This combined with Definition 2.5 and Theorems 2.4 and 2.15 gives the required result. □

Finally we have a brief look at minimal exposed faces, which will come in useful in Section 7.

Theorem 2.21. *If $\mathcal{K}$ is a proper cone, $x \in \operatorname{bd} \mathcal{K}$ and $a \in \operatorname{reint} \mathcal{F}(\mathcal{K}^*, x)$, then the minimal exposed face of $\mathcal{K}$ containing x is given by $\mathcal{F}(\mathcal{K}, a)$.*

Proof. Consider any exposed face $\mathcal{F}$ of $\mathcal{K}$ such that $x \in \mathcal{F}$. From Theorem 2.15 and Lemma 2.18 we see that there exists a $b \in \mathcal{F}(\mathcal{K}^*, x) \setminus \{0\}$ such that $\mathcal{F} = \mathcal{F}(\mathcal{K}, b)$. As $a \in \operatorname{reint} \mathcal{F}(\mathcal{K}^*, x)$ there also exists $\theta \in (0, 1)$, $c \in \mathcal{F}(\mathcal{K}^*, x) \setminus \{0\}$ such that $a = \theta b + (1 - \theta) c$. Now using Lemmas 2.16 and 2.19 we get that

$$\mathcal{F}(\mathcal{K}, a) = \mathcal{F}(\mathcal{K}, b) \cap \mathcal{F}(\mathcal{K}, c) \subseteq \mathcal{F}(\mathcal{K}, b) = \mathcal{F}.$$

Therefore all exposed faces of $\mathcal{K}$ containing x must also contain the exposed face $\mathcal{F}(\mathcal{K}, a)$ and so this must be the minimal exposed face. □

3. Copositive and completely positive cones

The results from the previous section are also true for proper cones in spaces which are isomorphic to the real space, for example the set of symmetric matrices, which is the space that the copositive and completely cones sit in.

We will now illustrate some of the theorems from the previous section with a quick example in Fig. 1. For this we use the copositive and complete positive cones in $\mathcal{S}^2$, which are proper cones and duals of each other. In order to show these in two dimensions we first use the svec operator to give an isomorphic mapping from $\mathcal{S}^2$ to $\mathbb{R}^3$.

$$\operatorname{svec}\left[\begin{pmatrix} x & y \\ y & z \end{pmatrix}\right] := (x \quad \sqrt{2} y \quad z)^{\mathsf{T}},$$

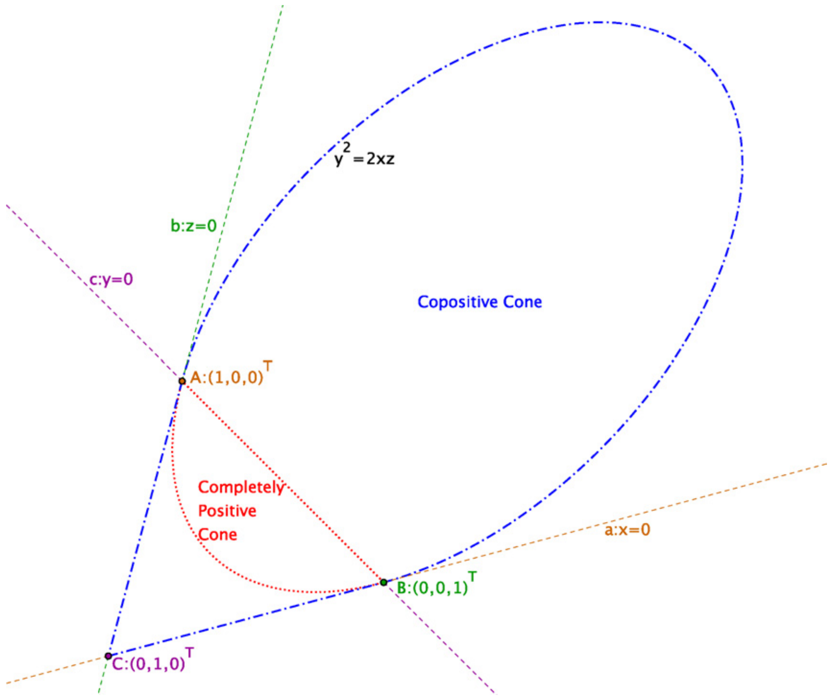

Fig. 1. The figure above is of bases of cones equivalent to the copositive and completely positive cones in $\mathcal{S}^2$, contained within "$- \cdot - \cdot -$" and "......" respectively. The equivalence between this figure and the cones is explained in Section 3. Letters in upper case label rays and the equivalent letters in lower case label the corresponding hyperplanes.

which has the property

$$\langle A, B\rangle = \operatorname{trace}(AB) = \operatorname{svec}(A)^{\mathsf{T}} \operatorname{svec}(B).$$

We then consider the bases of these cones given by their intersections with the hyperplane $e^{\mathsf{T}}x = 1$, where e is the all-ones vector.

For these cones we have the following relationships between their extreme rays and their exposed faces:

(i) A and B give exposed rays of the completely positive cone, whilst the corresponding hyperplanes a and b give maximal faces of the copositive cone.
(ii) A and B give extreme but not exposed rays of the copositive cone, whilst the corresponding hyperplanes a and b give nonmaximal faces of the completely positive cone.
(iii) C gives an exposed ray of the copositive cone, whilst the corresponding hyperplane c gives a maximal face of the completely positive cone.

4. Extreme rays of the copositive and completely positive cones

In this section we will look at extreme rays of the copositive and completely positive cones. We will show that for $n \geqslant 2$, every extreme ray of the completely positive cone is also an exposed ray of it, and this is in contrast to the copositive cone for which we will give an example of extreme rays which are not exposed.

Before we begin this we first introduce the following notation, which we will use regularly in this section, along with the corresponding properties, which are trivial to prove by the definitions.

Lemma 4.1. *For a finite set of vectors $\mathcal{Y}$, we define the matrix*

$$A(\mathcal{Y}) := \sum_{v\in\mathcal{Y}} vv^{\mathsf{T}}.$$

For a finite set $\mathcal{Y} \subset \mathbb{R}^n$ we have that $A(\mathcal{Y}) \in \mathcal{S}^n_+ \subset \mathcal{C}^n$, and the exposed face,

$$\mathcal{F}\big(\mathcal{C}^*, A(\mathcal{Y})\big) = \left\{ \sum_i c_i c_i^{\mathsf{T}} \;\middle|\; c_i \in \mathbb{R}^n_+,\ c_i^{\mathsf{T}} v = 0 \text{ for all } v \in \mathcal{Y},\ \text{for all } i \right\}.$$

For a finite set $\mathcal{Y} \subset \mathbb{R}^n_+$ we have that $A(\mathcal{Y}) \in \mathcal{C}^{*n}$, and the exposed face,

$$\mathcal{F}\big(\mathcal{C}, A(\mathcal{Y})\big) = \big\{X \in \mathcal{C} \;\big|\; v^\mathsf{T} X v = 0 \text{ for all } v \in \mathcal{Y}\big\}.$$

We will now consider the extreme rays of the completely positive cone.

Theorem 4.2. *For $n \geqslant 2$, every extreme ray of the completely positive cone is also an exposed ray of it, i.e.*

$$\operatorname{Exp}\big(\mathcal{C}^{*n}\big) = \operatorname{Ext}\big(\mathcal{C}^{*n}\big) = \big\{bb^\mathsf{T} \;\big|\; b \in \mathbb{R}^n_+ \backslash\{0\}\big\}.$$

Proof. The set of extreme rays of the completely positive cone is already known,

$$\operatorname{Ext}\big(\mathcal{C}^*\big) = \big\{bb^\mathsf{T} \;\big|\; b \in \mathbb{R}^n_+ \backslash\{0\}\big\} \quad \big(\text{see [1, p. 71]}\big).$$

For an arbitrary $b \in \mathbb{R}^n_+ \setminus \{0\}$, let $\mathcal{Y}_b$ be a set of $n-1$ linearly independent vectors which are perpendicular to b. Now consider the exposed face of the completely positive cone given by $A(\mathcal{Y}_b)$,

$$\begin{aligned}
\mathcal{F}\big(\mathcal{C}^*, A(\mathcal{Y}_b)\big) &= \left\{ \sum_i c_i c_i^\mathsf{T} \;\middle|\; c_i \in \mathbb{R}^n_+,\ c_i^\mathsf{T} v = 0 \text{ for all } v \in \mathcal{Y}_b,\ \text{for all } i \right\} \\
&= \left\{ \sum_i c_i c_i^\mathsf{T} \;\middle|\; c_i = \alpha_i b,\ \alpha_i \geqslant 0 \text{ for all } i \right\} \\
&= \big\{\alpha bb^\mathsf{T} \;\big|\; \alpha \geqslant 0\big\}.
\end{aligned}$$

Therefore the ray given by bb^T must be an exposed ray by the definition. □

For $n \geqslant 4$ finding the complete set of extreme rays of the copositive cone is still an open question. We do however have the following results for matrices which give the extreme rays.

Theorem 4.3. *For $n \geqslant 2$, we have the following results for the extreme rays of the copositive cone*:

- (i) $\alpha(e_i e_j^\mathsf{T} + e_j e_i^\mathsf{T}) \in \operatorname{Ext}(\mathcal{C}^n)$, *where $i, j = 1, \dots, n$, $\alpha > 0$, and this is all the nonnegative matrices which give extreme rays of copositive cone.*
- (ii) $aa^\mathsf{T} \in \operatorname{Ext}(\mathcal{C})$, *where $a \in \mathbb{R}^n \setminus (\mathbb{R}^n_+ \cup (-\mathbb{R}^n_+))$, and this, along with the relevant nonnegative matrices $\alpha e_i e_i^\mathsf{T}$ from* (i), *is all the positive semidefinite matrices which give extreme rays of copositive cone.*
- (iii) *The set $\{X \in \operatorname{Ext}(\mathcal{C}) \mid (X)_{ij} \in \{-1, 0, +1\},\ (X)_{ii} = +1$ for all $i, j\}$, was found in* [13].
- (iv) *$PDMDP^\mathsf{T} \in \operatorname{Ext}(\mathcal{C}) \Leftrightarrow M \in \operatorname{Ext}(\mathcal{C})$, where P is a permutation matrix and D is a diagonal matrix such that $(D)_{ii} > 0$ for all i.*
- (v) *For $M \in \mathcal{C}^n \setminus \{0\}$, $B \in \mathbb{R}^{n \times m}$ we have that $\left(\begin{smallmatrix} M & B \\ B^\mathsf{T} & 0 \end{smallmatrix}\right) \in \operatorname{Ext}(\mathcal{C}^{n+m})$ if and only if $B = 0$ and $M \in \operatorname{Ext}(\mathcal{C}^n)$.*
- (vi) *If $\left(\begin{smallmatrix} M & m \\ m^\mathsf{T} & \mu \end{smallmatrix}\right) \in \operatorname{Ext}(\mathcal{C}^n) \setminus \mathcal{N}^n$, then $\left(\begin{smallmatrix} M & m & m \\ m^\mathsf{T} & \mu & \mu \\ m^\mathsf{T} & \mu & \mu \end{smallmatrix}\right) \in \operatorname{Ext}(\mathcal{C}^{n+1})$.*

Proof. Where these results have an explicit reference we shall just give the reference rather than reproving the result. Parts (i) and (ii) come directly from [14]. Part (iii) is from [13]. Part (iv) is trivial to show by transforming the coordinate basis. Part (vi) comes directly from [15]. We are now left to prove part (v):

We let $\widehat{M} = \left(\begin{smallmatrix} M & B \\ B^\mathsf{T} & 0 \end{smallmatrix}\right)$.

From Theorem 1.1 we can see that $\widehat{M} \in \mathcal{C}^{n+m}$ if and only if $M \in \mathcal{C}^n$ and $B \geqslant 0$. We have that $\widehat{M}$ is the sum of the two copositive matrices.

$$\widehat{M} = \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & B \\ B^\mathsf{T} & 0 \end{pmatrix}.$$

Therefore $\widehat{M} \in \operatorname{Ext}(\mathcal{C})$ implies that $B = 0$.

The result now comes directly from [8,15]. □

We now give an example of an extreme ray of the copositive cone which is not an exposed ray.

Theorem 4.4. *Let $n \geqslant 2$ and $i \in \{1, \dots, n\}$. Then $e_i e_i^\mathsf{T}$ gives a ray of the copositive cone $\mathcal{C}^n$ which is extreme but not exposed.*

Proof. From the previous theorem we have that $e_i e_i^\mathsf{T} \in \operatorname{Ext}(\mathcal{C})$.

Assume by contradiction that $e_ie_i^\mathsf{T}$ also gives an exposed ray of the copositive cone. This is only true if there exists an exposed face of the copositive cone which is equal to this ray. Therefore, by Theorem 2.15, there must exist $B \in \mathcal{C}^*$ such that

$$\{\alpha e_ie_i^\mathsf{T} \mid \alpha \geqslant 0\} = \mathcal{F}(\mathcal{C}, B) := \{A \in \mathcal{C} \mid \langle A, B\rangle = 0\}.$$

As $B \in \mathcal{C}^*$, we decompose it as $B = \sum_k b_kb_k^\mathsf{T}$, where $b_k \in \mathbb{R}^n_+$ for all k.

As $e_ie_i^\mathsf{T} \in \mathcal{F}(\mathcal{C}, B)$, we get that $\langle e_ie_i^\mathsf{T}, B\rangle = 0$ and so $b_k^\mathsf{T}e_i = 0$ for all k.

We now consider the copositive matrix $(e_ie_j^\mathsf{T} + e_je_i^\mathsf{T})$, where $i \neq j$.

$$\langle e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}, B\rangle = 2\sum\nolimits_k (e_j^\mathsf{T}b_k)(b_k^\mathsf{T}e_i) = 0.$$

Therefore $(e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}) \in \mathcal{F}(\mathcal{C}, B) \setminus \{\alpha e_ie_i^\mathsf{T} \mid \alpha \geqslant 0\} = \emptyset$, a contradiction. $\square$

From the extension of Straszewicz's Theorem, we naturally have that the copositive cone does have exposed rays. Before we present some of these we will first need the following lemma for part of the proof.

Lemma 4.5. *For a matrix $X \in \mathcal{C}$ we have the following*:

(i) *If $(e_i + e_j)^\mathsf{T}X(e_i + e_j) = 0$ then $(X)_{ii} = (X)_{jj} = -(X)_{ij}$.*
(ii) *If $(X)_{ii} = (X)_{jj} = (X)_{kk} = -(X)_{ij} = -(X)_{jk}$ and we also have that $(e_i + 2e_j + e_k)^\mathsf{T}X(e_i + 2e_j + e_k) = 0$ then $(X)_{ik} = (X)_{ii}$.*

Proof. Part (ii) is trivial to show.

Part (i) comes from the inequality of arithmetic and geometric means and some of the properties of copositive matrices from Theorem 1.1, namely as $X \in \mathcal{C}$ we have that $(X)_{ij} \geqslant -\sqrt{(X)_{ii}(X)_{jj}}$ for all i, j and $(X)_{ii} \geqslant 0$ for all i.

$$\begin{aligned} 0 &= (e_i + e_j)^\mathsf{T}X(e_i + e_j) \\ &= (X)_{ii} + (X)_{jj} + 2(X)_{ij} \\ &\geqslant (X)_{ii} + (X)_{jj} - 2\sqrt{(X)_{ii}(X)_{jj}} \\ &\geqslant 0. \end{aligned}$$

Thereby we have that $(X)_{ii} = (X)_{jj} = \sqrt{(X)_{ii}(X)_{jj}} = -(X)_{ij}$. $\square$

Theorem 4.6. *For $n \geqslant 2$, we have the following results for the exposed rays of the copositive cone*:

(i) *$\alpha(e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}) \in \mathrm{Exp}(\mathcal{C}^n)$, where $i \neq j$, $\alpha > 0$.*
(ii) *$aa^\mathsf{T} \in \mathrm{Exp}(\mathcal{C}^n)$, where $a \in \mathbb{R}^n \setminus (\mathbb{R}^n_+ \cup (-\mathbb{R}^n_+))$.*
(iii) *$M \in \mathrm{Exp}(\mathcal{C}^n)$ for all $M \in \mathrm{Ext}(\mathcal{C}^n)$ such that $(M)_{ij} = \pm 1$ for all i, j.*
(iv) *$PDMDP^\mathsf{T} \in \mathrm{Exp}(\mathcal{C}^n) \Leftrightarrow M \in \mathrm{Exp}(\mathcal{C}^n)$, where P is a permutation matrix and D is a diagonal matrix such that $(D)_{ii} > 0$ for all i.*
(v) *$\widehat{M} = \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix} \in \mathrm{Exp}(\mathcal{C}^{n+m})$ if and only if $M \in \mathrm{Exp}(\mathcal{C}^n)$.*
(vi) *If $\begin{pmatrix} M & m \\ m^\mathsf{T} & \mu \end{pmatrix} \in \mathrm{Exp}(\mathcal{C}^n) \setminus \mathcal{N}^n$, then $\begin{pmatrix} M & m & m \\ m^\mathsf{T} & \mu & \mu \\ m^\mathsf{T} & \mu & \mu \end{pmatrix} \in \mathrm{Exp}(\mathcal{C}^{n+1})$.*

Proof. In this proof we will regularly use Theorem 2.15 and Lemma 4.1.

(i) For an arbitrary $i \neq j$, $i, j = 1, \dots, n$ we define the set

$$\mathcal{Y}_{i,j} := \{e_k + e_l \mid k \leqslant l,\ \{k, l\} \neq \{i, j\}\} \subset \mathbb{R}^n_+.$$

Now we consider the exposed face of the copositive cone given by $A(\mathcal{Y}_{i,j})$,

$$\begin{aligned} \mathcal{F}(\mathcal{C}, A(\mathcal{Y}_{i,j})) &= \{X \in \mathcal{C} \mid (e_k + e_l)^\mathsf{T}X(e_k + e_l) = 0 \text{ for all } \{k, l\} \neq \{i, j\}\} \\ &= \{X \in \mathcal{C} \mid (X)_{kk} + 2(X)_{kl} + (X)_{ll} = 0 \text{ for all } \{k, l\} \neq \{i, j\}\} \\ &= \{X \in \mathcal{C} \mid (X)_{kl} = 0 \text{ for all } \{k, l\} \neq \{i, j\}\} \quad \text{(by first considering } k = l) \\ &= \{\alpha(e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}) \mid \alpha \geqslant 0\}. \end{aligned}$$

Therefore this ray must be an exposed ray by the definition.

(ii) For an arbitrary $a \in \mathbb{R}^n \setminus (\mathbb{R}^n_+ \cup (-\mathbb{R}^n_+))$ we start by defining the following.

$$\mathcal{I}_+ := \{ i \mid (a)_i > 0 \} \neq \emptyset,$$
$$\mathcal{I}_0 := \{ i \mid (a)_i = 0 \},$$
$$\mathcal{I}_- := \{ i \mid (a)_i < 0 \} \neq \emptyset,$$
$$b := \frac{1}{|\mathcal{I}_+|} \sum_{i \in \mathcal{I}_+} \frac{1}{(a)_i} e_i + \frac{1}{|\mathcal{I}_-|} \sum_{i \in \mathcal{I}_-} \frac{1}{|(a)_i|} e_i + \sum_{i \in \mathcal{I}_0} e_i,$$

and for arbitrary $i_+ \in \mathcal{I}_+$, $i_- \in \mathcal{I}_-$,

$$\mathcal{Y}_a := \{ e_j \mid j \in \mathcal{I}_0 \} \cup \left\{ \frac{1}{(a)_{i_+}} e_{i_+} + \frac{1}{|(a)_j|} e_j \;\middle|\; j \in \mathcal{I}_- \right\} \cup \left\{ \frac{1}{(a)_j} e_j + \frac{1}{|(a)_{i_-}|} e_{i_-} \;\middle|\; j \in \mathcal{I}_+ \setminus \{i_+\} \right\}.$$

It is immediately apparent that b is strictly positive, $\mathcal{Y}_a \subseteq \mathbb{R}^n_+$, and for all $v \in \mathcal{Y}_a \cup \{b\}$ we have that $v^{\mathsf{T}} a = 0$. It can also be seen that $\mathcal{Y}_a$ is a set of $n-1$ linearly independent vectors. We now consider the exposed face of the copositive cone given by $A(\mathcal{Y}_a \cup \{b\})$,

$$\begin{aligned}
\mathcal{F}(\mathcal{C}, A(\mathcal{Y}_a \cup \{b\})) &= \{ X \in \mathcal{C} \mid b^{\mathsf{T}} X b = 0,\ v^{\mathsf{T}} X v = 0 \text{ for all } v \in \mathcal{Y}_a \} \\
&= \{ X \in \mathcal{S}_+ \mid b^{\mathsf{T}} X b = 0,\ v^{\mathsf{T}} X v = 0 \text{ for all } v \in \mathcal{Y}_a \} \quad \big(\text{from Theorem 1.1 and the fact that } b \in \mathbb{R}^n_{++}\big) \\
&= \left\{ \sum_i c_i c_i^{\mathsf{T}} \;\middle|\; c_i \in \mathbb{R}^n,\ c_i^{\mathsf{T}} v = 0 \begin{array}{l} \text{for all } v \in \mathcal{Y}_a \cup \{b\}, \\ \text{for all } i \end{array} \right\} \\
&= \left\{ \sum_i c_i c_i^{\mathsf{T}} \;\middle|\; \beta \in \mathbb{R},\ c_i = \beta a \text{ for all } i \right\} \\
&= \{ \alpha a a^{\mathsf{T}} \mid \alpha \geqslant 0 \}.
\end{aligned}$$

Therefore the ray given by aa^{T} must be an exposed ray by the definition.

(iii) A method for finding all the matrices M giving extreme rays of the copositive cone with $(M)_{ij} = \pm 1$ for all i, j was first presented in [16], however we will use the more general method from [13]. In this they defined the simple graphs $G_1(M)$ and $G_{-1}(M)$ associated with a symmetric matrix M such that $(M)_{ij} = \pm 1$ for all i, j and $(M)_{ii} = 1$ for all i. $G_1(M)$ ($G_{-1}(M)$) is defined to be a graph on n vertices such that i and j are adjacent if $(M)_{ij} = 1$ ($(M)_{ij} = -1$). We have that M gives an extreme ray of the copositive cone if and only if $G_{-1}(M)$ is connected and contains no triangles, and $G_1(M)$ is precisely the edges (i, j) such that i and j are at a distance of 2 in $G_{-1}(M)$.

Now for an arbitrary matrix M of this form we define the following,

$$\mathcal{J}_- := \{ (i, j) \mid i < j,\ (M)_{ij} = -1 \},$$
$$\mathcal{J}_\pm := \{ (i, j, k) \mid i < k,\ (M)_{ik} = -(M)_{ij} = -(M)_{jk} = 1 \},$$
$$\mathcal{Y}_- := \{ e_i + e_j \mid (i, j) \in \mathcal{J}_- \},$$
$$\mathcal{Y}_\pm := \{ e_i + 2e_j + e_k \mid (i, j, k) \in \mathcal{J}_\pm \}.$$

Now we consider the exposed face of the copositive cone given by the completely positive matrix $A(\mathcal{Y}_\pm \cup \mathcal{Y}_-)$,

$$\begin{aligned}
\mathcal{F}(\mathcal{C}, A(\mathcal{Y}_\pm \cup \mathcal{Y}_-)) &= \{ X \in \mathcal{C} \mid v^{\mathsf{T}} X v = 0 \text{ for all } v \in \mathcal{Y}_\pm \cup \mathcal{Y}_- \} \\
&= \left\{ X \in \mathcal{C} \;\middle|\; \begin{array}{l} v^{\mathsf{T}} X v = 0 \text{ for all } v \in \mathcal{Y}_\pm, \\ \alpha \geqslant 0,\ (X)_{ii} = \alpha \text{ for all } i, \\ (X)_{jk} = -\alpha \text{ for all } (j, k) \in \mathcal{J}_- \end{array} \right\} \\
&\qquad \big(\text{from Lemma 4.5(i) and because } G_{-1}(M) \text{ is connected}\big) \\
&= \{ \alpha M \mid \alpha \geqslant 0 \} \quad \big(\text{from Lemma 4.5(ii) and the condition on } G_1(M)\big).
\end{aligned}$$

Therefore the ray given by M must be an exposed ray by the definition.

(iv) The multiplications with a permutation matrix P and a diagonal matrix D with all the diagonal entries strictly positive can be seen as a transformation of the coordinate basis, and as $DP^{\mathsf{T}} \mathbb{R}^n_+ = \mathbb{R}^n_+$ the implications are trivial.

(v) ($\Rightarrow$) If $\widehat{M} \in \operatorname{Exp}(\mathcal{C}^{n+m})$ then there exists a $\widehat{B} \in \mathcal{C}^*$ such that the exposed face $\mathcal{F}(\mathcal{C}, \widehat{B}) = \{ \alpha \widehat{M} \mid \alpha \geqslant 0 \}$. As $\widehat{B}$ is completely positive there must exist sets $\{b_1, \dots, b_p\} \subset \mathbb{R}^n_+$ and $\{\beta_1, \dots, \beta_p\} \subset \mathbb{R}^m_+$ such that

$$\widehat{B} = \sum_i \begin{pmatrix} b_i \\ \beta_i \end{pmatrix} \begin{pmatrix} b_i \\ \beta_i \end{pmatrix}^{\mathsf{T}}.$$

If we now define $B = \sum_i b_i b_i^{\mathsf{T}}$ it can be seen that the exposed face $\mathcal{F}(\mathcal{C}, B) = \{ \alpha M \mid \alpha \geqslant 0 \}$.

($\Leftarrow$) For the case when $M \in \mathrm{Exp}(\mathcal{C}) \cap \mathcal{S}_+$, it is trivial that $\widehat{M} \in \mathrm{Exp}(\mathcal{C})$, by considering Theorem 4.3(ii), Theorem 4.4 and Theorem 4.6(ii).

Now we consider the case when $M \in \mathrm{Exp}(\mathcal{C}) \setminus \mathcal{S}_+$. As M is an exposed ray there must exist a $B_M \in \mathcal{C}^{*n}$ such that $\mathcal{F}(\mathcal{C}, B_M) = \{\alpha M \mid \alpha \geqslant 0\}$ and as B_M is completely positive there must exist a set $\{b_1, \dots, b_p\} \subset \mathbb{R}^n_+$ such that $B_M = \sum_i b_i b_i^\mathsf{T}$. These vectors must span the entire space, otherwise there exists an $a \in \mathbb{R}^n \setminus \{0\}$ such that $a^\mathsf{T} b_i = 0$ for all i which would imply that $aa^\mathsf{T} \in \mathcal{F}(\mathcal{C}, B_M) \cap \mathcal{S}_+$. Now we define the following matrices in $\mathcal{C}^{*(n+m)}$,

$$\begin{aligned}
\widehat{B}_1 &:= \sum_{i=1}^{p} \begin{pmatrix} b_i \\ 0 \end{pmatrix} \begin{pmatrix} b_i \\ 0 \end{pmatrix}^\mathsf{T} = \begin{pmatrix} B_M & 0 \\ 0 & 0 \end{pmatrix}, \\
\widehat{B}_2 &:= \sum_{j,k=1}^{m} \begin{pmatrix} 0 \\ e_j + e_k \end{pmatrix} \begin{pmatrix} 0 \\ e_j + e_k \end{pmatrix}^\mathsf{T}, \\
\widehat{B}_3 &:= \sum_{i=1}^{p} \sum_{j=1}^{m} \begin{pmatrix} b_i \\ e_j \end{pmatrix} \begin{pmatrix} b_i \\ e_j \end{pmatrix}^\mathsf{T}, \\
\widehat{B}_4 &:= \widehat{B}_1 + \widehat{B}_2 + \widehat{B}_3,
\end{aligned}$$

and consider the exposed face of $\mathcal{C}^{n+m}$ given by $\widehat{B}_4$,

$$\begin{aligned}
\mathcal{F}(\mathcal{C}, \widehat{B}_4) &= \left\{ \begin{pmatrix} X & Y \\ Y^\mathsf{T} & Z \end{pmatrix} \in \mathcal{C} \;\middle|\; \left\langle \widehat{B}_1 + \widehat{B}_2 + \widehat{B}_3, \begin{pmatrix} X & Y \\ Y^\mathsf{T} & Z \end{pmatrix} \right\rangle = 0 \right\} \\
&= \left\{ \begin{pmatrix} X & Y \\ Y^\mathsf{T} & Z \end{pmatrix} \in \mathcal{C} \;\middle|\; \left\langle \widehat{B}_l, \begin{pmatrix} X & Y \\ Y^\mathsf{T} & Z \end{pmatrix} \right\rangle = 0,\ l = 1, 2, 3 \right\} \\
&= \left\{ \begin{pmatrix} X & Y \\ Y^\mathsf{T} & Z \end{pmatrix} \in \mathcal{C} \;\middle|\; \begin{array}{l} \langle B_M, X \rangle = 0, \\ (Z)_{jj} + (Z)_{kk} + 2(Z)_{jk} = 0 \text{ for all } j, k, \\ b_i^\mathsf{T} X b_i + (Z)_{jj} + 2 b_i^\mathsf{T} Y e_j = 0 \text{ for all } i, j \end{array} \right\} \\
&= \left\{ \begin{pmatrix} \alpha M & Y \\ Y^\mathsf{T} & 0 \end{pmatrix} \in \mathcal{C} \;\middle|\; \alpha \geqslant 0,\ Y e_j = 0 \text{ for all } j \right\} \\
&= \{\alpha \widehat{M} \mid \alpha \geqslant 0\}.
\end{aligned}$$

Therefore this must be an exposed ray by the definition.

(vi) If $\left(\begin{smallmatrix} M & m \\ m^\mathsf{T} & \mu \end{smallmatrix}\right) \in \mathcal{C}$ and $M = 0$ then we get that both m and μ must be nonnegative, and thereby the whole matrix must be nonnegative, contradicting the given constraints. Therefore we must have that $M \in \mathcal{C} \setminus \{0\}$.

If $\left(\begin{smallmatrix} M & m \\ m^\mathsf{T} & \mu \end{smallmatrix}\right)$ gives an exposed ray of the copositive cone then there must exist a $B \in \mathcal{C}^{*n}$ such that

$$\left\{ \alpha \begin{pmatrix} M & m \\ m^\mathsf{T} & \mu \end{pmatrix} \;\middle|\; \alpha \geqslant 0 \right\} = \mathcal{F}(\mathcal{C}, B) := \left\{ X \in \mathcal{C} \mid \langle B, X \rangle = 0 \right\}.$$

As B is completely positive there must exist sets $\{b_1, \dots, b_k\} \subset \mathbb{R}^{n-1}_+$ and $\{\beta_1, \dots, \beta_k\} \subset \mathbb{R}_+$ such that

$$B = \sum_i \begin{pmatrix} b_i \\ \beta_i \end{pmatrix} \begin{pmatrix} b_i \\ \beta_i \end{pmatrix}^\mathsf{T}.$$

We now consider the following finite sets in $\mathbb{R}^n_+$,

$$\begin{aligned}
\mathcal{Y}_1 &= \left\{ \begin{pmatrix} b_1 \\ \beta_1 \\ 0 \end{pmatrix}, \dots, \begin{pmatrix} b_k \\ \beta_k \\ 0 \end{pmatrix} \right\}, \\
\mathcal{Y}_2 &= \left\{ \begin{pmatrix} b_1 \\ 0 \\ \beta_1 \end{pmatrix}, \dots, \begin{pmatrix} b_k \\ 0 \\ \beta_k \end{pmatrix} \right\}, \\
\mathcal{Y}_3 &= \left\{ \begin{pmatrix} 2b_1 \\ \beta_1 \\ \beta_1 \end{pmatrix}, \dots, \begin{pmatrix} 2b_k \\ \beta_k \\ \beta_k \end{pmatrix} \right\},
\end{aligned}$$

and the exposed face of $\mathcal{C}^{(n+1)}$ given by $A(\mathcal{Y}_1 \cup \mathcal{Y}_2 \cup \mathcal{Y}_3)$,

$$\begin{aligned}
\mathcal{F}\big(\mathcal{C}, A(\mathcal{Y}_1 \cup \mathcal{Y}_2 \cup \mathcal{Y}_3)\big) &:= \left\{\widehat{X} \in \mathcal{C}^{n+1} \;\middle|\; v^\mathsf{T}\widehat{X}v = 0 \begin{array}{l}\text{for all } v \in \mathcal{Y}_i,\\ \text{for all } i\end{array}\right\} \\
&= \left\{\begin{pmatrix} X & x_1 & x_2 \\ x_1^\mathsf{T} & \gamma_1 & \zeta \\ x_2^\mathsf{T} & \zeta & \gamma_2 \end{pmatrix} \in \mathcal{C} \;\middle|\; v^\mathsf{T}\begin{pmatrix} X & x_1 & x_2 \\ x_1^\mathsf{T} & \gamma_1 & \zeta \\ x_2^\mathsf{T} & \zeta & \gamma_2 \end{pmatrix} v = 0, \begin{array}{l}\text{for all } v \in \mathcal{Y}_i,\\ \text{for all } i\end{array}\right\} \\
&= \left\{\begin{pmatrix} X & x_1 & x_2 \\ x_1^\mathsf{T} & \gamma_1 & \zeta \\ x_2^\mathsf{T} & \zeta & \gamma_2 \end{pmatrix} \in \mathcal{C} \;\middle|\; \begin{array}{l} \left\langle B, \begin{pmatrix} X & x_j \\ x_j^\mathsf{T} & \gamma_j \end{pmatrix}\right\rangle = 0,\ j = 1, 2, \\ \left\langle B, \begin{pmatrix} 4X & 2(x_1 + x_2) \\ 2(x_1 + x_2)^\mathsf{T} & \gamma_1 + \gamma_2 + 2\zeta \end{pmatrix}\right\rangle = 0 \end{array}\right\} \\
&= \left\{\alpha\begin{pmatrix} M & m & m \\ m^\mathsf{T} & \mu & \mu \\ m^\mathsf{T} & \mu & \mu \end{pmatrix} \in \mathcal{C} \;\middle|\; \alpha \geqslant 0\right\}.
\end{aligned}$$

The last line is in part implied by the fact that we must have $M \neq 0$. We now have that this must be an exposed ray by the definition. □

5. Maximal faces of the copositive cone

We can now use results developed in this paper to give us the maximal faces of the copositive cone.

Lemma 5.1. *$\mathcal{F}$ is a maximal face of the copositive cone if and only if there exists $v \in \mathbb{R}^n_+ \setminus \{0\}$ such that*

$$\mathcal{F} = \mathcal{M}^n(v) := \{X \in \mathcal{C}^n \mid v^\mathsf{T}Xv = 0\}.$$

Proof. By Theorems 2.17, 2.20 and 4.2. □

We will now investigate the dimension of these faces. Without loss of generality we consider a vector defining a maximal face with the first p entries positive and the next $(n-p)$ entries equal to zero, for some $p \in \{1, \ldots, n\}$. We can do this as for any nonzero vector the coordinate basis can easily be permuted so that this is so.

Lemma 5.2. *Let $v = \binom{\hat{v}}{0} \in \mathbb{R}^n_+$, where $\hat{v} \in \mathbb{R}^p_{++}$ and $p \in \{1, \ldots, n\}$. Then*

$$\dim \mathcal{M}^n(v) = \dim \mathcal{M}^p(\hat{v}) + \frac{1}{2}(n-p)(n+p+1).$$

Proof. In this proof we will subdivide the matrices as follows:

$$A = \begin{pmatrix} Y & W^\mathsf{T} \\ W & Z \end{pmatrix} \in \mathcal{S}^n$$

such that

$$\begin{aligned}
&Y \in \mathcal{S}^p, \\
&W \in \mathbb{R}^{(n-p)\times p}, \\
&Z \in \mathcal{S}^{(n-p)}.
\end{aligned}$$

If A is copositive then Y and Z are copositive from Theorem 1.1.

$$\begin{aligned}
\mathcal{M}^n(v) &= \{A \in \mathcal{C}^n \mid v^\mathsf{T}Av = 0\} \\
&= \left\{A = \begin{pmatrix} Y & W^\mathsf{T} \\ W & Z \end{pmatrix} \in \mathcal{C}^n \;\middle|\; \hat{v}^\mathsf{T}Y\hat{v} = 0\right\} \\
&= \left\{A = \begin{pmatrix} Y & W^\mathsf{T} \\ W & Z \end{pmatrix} \in \mathcal{C}^n \;\middle|\; Y \in \mathcal{M}^p(\hat{v})\right\}.
\end{aligned}$$

To get an equation for the dimension of $\mathcal{M}^n(v)$, we will sandwich it between two other sets.

$$\mathcal{M}^n(v) \subseteq \left\{A = \begin{pmatrix} Y & W^\mathsf{T} \\ W & Z \end{pmatrix} \in \mathcal{S}^n \;\middle|\; \begin{array}{l} Y \in \mathcal{M}^p(\hat{v}), \\ Z \in \mathcal{C}^{(n-p)}, \end{array} W \in \mathbb{R}^{(n-p)\times p}\right\}.$$

Therefore,

$$\begin{aligned}\dim \mathcal{M}^n(v) &\leqslant \dim \mathcal{M}^p(\hat{v}) + \dim \mathcal{C}^{(n-p)} + \dim \mathbb{R}^{(n-p)\times p} \\ &= \dim \mathcal{M}^p(\hat{v}) + \frac{1}{2}(n-p)(n-p+1) + (n-p)p,\end{aligned}$$

$$\mathcal{M}^n(v) \supseteq \left\{ A = \begin{pmatrix} Y & W^\mathsf{T} \\ W & Z \end{pmatrix} \in \mathcal{S}^n \;\middle|\; \begin{array}{l} Y \in \mathcal{M}^p(\hat{v}), \\ Z \in \mathcal{C}^{(n-p)}, \end{array} \; W \in \mathbb{R}_+^{(n-p)\times p} \right\}.$$

Therefore,

$$\begin{aligned}\dim \mathcal{M}^n(v) &\geqslant \dim \mathcal{M}^p(\hat{v}) + \dim \mathcal{C}^{(n-p)} + \dim \mathbb{R}_+^{(n-p)\times p} \\ &= \dim \mathcal{M}^p(\hat{v}) + \frac{1}{2}(n-p)(n-p+1) + (n-p)p. \qquad \square\end{aligned}$$

We now need the dimension of $\mathcal{M}^p(\hat{v})$, which we can find using the following lemma.

Lemma 5.3. *Let $\{u_1, \dots, u_m\} \subset \mathbb{R}_+^p \setminus \{0\}$ be a set of linearly independent vectors, where $u_1 \in \mathbb{R}_{++}^p$ and $m < p$. Then we have that $\bigcap_{i=1}^m \mathcal{M}^p(u_i)$ is an exposed face of the copositive cone which is isomorphic to the positive semidefinite cone $\mathcal{S}_+^{(p-m)}$.*

Proof. It is easy to see that the intersection of exposed faces is another exposed face. From the conditions given we have that

$$\begin{aligned}\bigcap_{i=1}^m \mathcal{M}^p(u_i) &= \left\{ A \in \mathcal{C}^p \;\middle|\; u_i^\mathsf{T} A u_i = 0 \text{ for all } i = 1, \dots, m \right\} \\ &= \left\{ A \in \mathcal{S}_+^p \;\middle|\; u_i^\mathsf{T} A u_i = 0 \text{ for all } i = 1, \dots, m \right\} \quad \text{(from Theorem 1.1)} \\ &= \left\{ \sum_j a_j a_j^\mathsf{T} \;\middle|\; a_j \in \mathbb{R}^p,\ a_j^\mathsf{T} u_i = 0 \text{ for all } i, j \right\}.\end{aligned}$$

This set can now be seen to be isomorphic to $\mathcal{S}_+^{(p-m)}$. $\square$

We now use this to get the dimensions of the maximal faces.

Lemma 5.4. *Let $v = \binom{\hat{v}}{0} \in \mathbb{R}_+^n$, where $\hat{v} \in \mathbb{R}_{++}^p$ and $p \in \{1, \dots, n\}$. Then*

$$\dim \mathcal{M}^n(v) = \frac{1}{2}n(n+1) - p.$$

Proof. From Lemma 5.2 we have that

$$\dim \mathcal{M}^n(v) = \dim \mathcal{M}^p(\hat{v}) + \frac{1}{2}(n-p)(n+p+1).$$

The previous lemma and $\hat{v} \in \mathbb{R}_{++}^p$ implies that $\mathcal{M}^p(\hat{v})$ is isomorphic to $\mathcal{S}_+^{p-1}$, so $\dim \mathcal{M}^p(\hat{v}) = \dim \mathcal{S}_+^{p-1} = \frac{1}{2}p(p-1)$. Consequently,

$$\dim \mathcal{M}^n(v) = \frac{1}{2}p(p-1) + \frac{1}{2}(n-p)(n+p+1) = \frac{1}{2}n(n+1) - p. \qquad \square$$

By considering permutations of the coordinate basis we can now generalise the result from the previous lemma for all $v \in \mathbb{R}_+^n \setminus \{0\}$ and combine this with Lemma 5.1 in order to give us the following theorem on the maximal faces of the copositive cone.

Theorem 5.5. *$\mathcal{F}$ is a maximal face of the copositive cone if and only if there exists $v \in \mathbb{R}_+^n \setminus \{0\}$ such that*

$$\mathcal{F} = \mathcal{M}^n(v) := \left\{ X \in \mathcal{C}^n \;\middle|\; v^\mathsf{T} X v = 0 \right\}.$$

For a vector $v \in \mathbb{R}_+^n \setminus \{0\}$ with p nonzero entries,

$$\dim \mathcal{M}^n(v) = \frac{1}{2}n(n+1) - p.$$

An interesting result from this is that we get the following tight inequalities for the dimension of a maximal face $\mathcal{M}$ of the copositive cone $\mathcal{C}^n$,

$$\dim \mathcal{C}^{(n-1)} \leqslant \dim \mathcal{M} \leqslant \dim \mathcal{C}^n - 1.$$

We can now show that the copositive cone has facets, as defined in Definition 2.1.

Theorem 5.6. *For $n \geqslant 2$, the copositive cone $\mathcal{C}^n$ has n facets and they are of the following form,*

$$\mathcal{M}^n(e_i) = \{A \in \mathcal{C}^n \mid (A)_{ii} = 0\} \quad \text{for } i = 1, \ldots, n,$$
$$\mathcal{M}^n(e_1) = \left\{ \begin{pmatrix} 0 & b^\mathsf{T} \\ b & B \end{pmatrix} \,\middle|\, b \geqslant 0,\ B \in \mathcal{C}^{(n-1)} \right\}.$$

(*When being more specific about the form we took $i = 1$ for simplicity. The result can then be extended by permuting the coordinate basis.*)

Proof. From Theorem 5.5 it can be clearly seen that the facets of the copositive cone are produced by vectors with only one nonzero entry. It can also be clearly seen that multiplying a vector by a strictly positive constant does not change the face that it describes, thereby all the facets can be produced by the unit vectors e_i for $i = 1, \ldots, n$. Using this we now get the following as the facets.

$$\mathcal{M}^n(e_i) = \{A \in \mathcal{C}^n \mid e_i^\mathsf{T} A e_i = 0\} = \{A \in \mathcal{C}^n \mid (A)_{ii} = 0\},$$
$$\dim \mathcal{M}^n(e_i) = \frac{1}{2}n(n+1) - 1 = \dim \mathcal{C}^n - 1.$$

In order to be more specific about the form that the facets take we first note that the conditions we give in the form are obviously sufficient for the matrix being on the face. Using Theorem 1.1 we see that these conditions are also necessary. □

6. Maximal faces of the completely positive cone

We were able to find all the maximal faces of the copositive cone due to the fact that we know all the extreme rays of the completely positive cone. Unfortunately finding the complete set of extreme rays for the copositive cone when $n \geqslant 4$ is still an open question. We can however consider some of the extreme rays which we do know. In particular, by Theorem 2.20, the exposed rays in Theorem 4.6 must give maximal faces of the completely positive cone. In [17] the authors consider the exposed face of the completely positive cone given by the Horn matrix and as this matrix is in the set $\{X \in \mathrm{Ext}(\mathcal{C}^5) \mid (X)_{ij} = \pm 1 \text{ for all } i\}$ we now see that the face is a maximal face. In this section we will look at some more maximal faces of the completely positive cone, although we start by presenting the following theorem for a general face of the completely positive cone. This theorem is trivial to prove by transforming the coordinate basis.

Theorem 6.1. *Let M be a copositive matrix, P be a permutation matrix and D be a diagonal matrix such that $(D)_{ii} > 0$ for all i, then*

$$\dim\bigl(\mathcal{F}\bigl(\mathcal{C}^*, PDMDP^\mathsf{T}\bigr)\bigr) = \dim\bigl(\mathcal{F}\bigl(\mathcal{C}^*, M\bigr)\bigr).$$

Before we start looking specifically at maximal faces of the completely positive cone we first need the following lemma.

Lemma 6.2. *If $\mathcal{Y} = \{v_1, \ldots, v_m\}$ is a set of linearly independent vectors, then the following is a set of $\frac{1}{2}m(m+1)$ linearly independent matrices,*

$$\mathcal{U} = \{(v_i + v_j)(v_i + v_j)^\mathsf{T} \mid i \leqslant j,\ i, j = 1, \ldots, m\}.$$

Proof. Suppose by contradiction that $\mathcal{U}$ is not a linearly independent set. Then there exists $\alpha \in \mathcal{S} \setminus \{0\}$ such that

$$0 = \frac{1}{2}\sum_{i,j}(\alpha)_{ij}(v_i + v_j)(v_i + v_j)^\mathsf{T} = \sum_i v_i \sum_j (\alpha)_{ij}(v_i + v_j)^\mathsf{T}.$$

As $\mathcal{Y}$ is a linearly independent set, we must have that for all i,

$$0 = \sum_j (\alpha)_{ij}(v_i + v_j)^\mathsf{T} = \left(\sum_j (\alpha)_{ij} + (\alpha)_{ii}\right) v_i^\mathsf{T} + \sum_{j \neq i} (\alpha)_{ij} v_j^\mathsf{T}.$$

Again as $\mathcal{Y}$ is a linearly independent set, we get that $(\alpha)_{ij} = 0$ for all i, j. □

We are now able to find the dimension of the maximal faces of the completely positive cone given by aa^T, where $a \in \mathbb{R}^n \setminus (\mathbb{R}^n_+ \cup (-\mathbb{R}^n_+))$.

Theorem 6.3. *Let $a \in \mathbb{R}^n \setminus (\mathbb{R}^n_+ \cup (-\mathbb{R}^n_+))$. Then $\mathcal{F}(\mathcal{C}^*, aa^\mathsf{T})$ is a maximal face of $\mathcal{C}^{*n}$ with dimension $\frac{1}{2}n(n-1)$.*

Proof. From Theorems 2.20 and 4.6 it can be immediately seen that $\mathcal{F}(\mathcal{C}^*, aa^\mathsf{T})$ is a maximal face of $\mathcal{C}^{*n}$.

From the decomposition of completely positive matrices we have,

$$\mathcal{F}\big(\mathcal{C}^*, aa^\mathsf{T}\big) := \big\{X \in \mathcal{C}^* \bigm| \langle X, aa^\mathsf{T}\rangle = 0\big\} = \left\{ \sum_i b_i b_i^\mathsf{T} \Bigm| b_i \in \mathbb{R}^n_+,\ b_i^\mathsf{T} a = 0 \text{ for all } i \right\}.$$

We now define $\mathcal{Y}_a$ as in the proof of Theorem 4.6(ii) and let

$$\mathcal{U} := \big\{(u+v)(u+v)^\mathsf{T} \bigm| u, v \in \mathcal{Y}_a\big\},$$
$$\mathcal{V} := \left\{ \sum_i b_i b_i^\mathsf{T} \Bigm| b_i \in \mathbb{R}^n,\ b_i^\mathsf{T} a = 0 \text{ for all } i \right\}.$$

It is not difficult to see that $\mathcal{U} \subset \mathcal{F}(\mathcal{C}^*, aa^\mathsf{T}) \subset \mathcal{V}$. $\mathcal{V}$ is isomorphic to $\mathcal{S}_+^{(n-1)}$, meaning that $\dim \mathcal{V} = \frac{1}{2}n(n-1)$, and therefore the dimension of the face must be less than or equal to this. It can also be seen that $\mathcal{Y}_a$ is a set of $n-1$ linearly independent vectors and so from the previous lemma we see that $\mathcal{U}$ gives us a set of $\frac{1}{2}n(n-1)$ linearly independent matrices contained in the face. □

Before we continue to consider more maximal faces we first need the following lemma which gives an upper bound on the dimension of an exposed face of the completely positive cone.

Lemma 6.4. *Let $\emptyset \neq \mathcal{I} \subseteq \{1, \dots, n\}$ and let $X \in \mathcal{C}^n$ such that $(X)_{ii} > 0$ for all $i \in \mathcal{I}$. Then*

$$\dim\big(\mathcal{F}\big(\mathcal{C}^{*n}, X\big)\big) \leqslant \frac{1}{2}n(n+1) - |\mathcal{I}| = \dim \mathcal{C}^{*n} - |\mathcal{I}|.$$

Proof. In this proof, for simplicity of notation, we let $\dim(\mathcal{F}(\mathcal{C}^{*n}, X)) = m$.

If we consider the diagonal matrix $D_{\pm\delta,i} := I \pm \delta e_i e_i^\mathsf{T}$ for $0 < \delta < 1$ then from Theorem 1.1 we have that the following matrix is copositive,

$$\begin{aligned} D_{\pm\delta,i} X D_{\pm\delta,i} &= X \pm \delta \widetilde{X}_i + \delta^2 \widehat{X}_i, \\ \text{where } \widetilde{X}_i &:= e_i e_i^\mathsf{T} X + X e_i e_i^\mathsf{T}, \\ \widehat{X}_i &:= (X)_{ii} e_i e_i^\mathsf{T}. \end{aligned}$$

As $(X)_{ii} > 0$ for all $i \in \mathcal{I}$, we have that $\{\widetilde{X}_i \mid i \in \mathcal{I}\}$ is a set of $|\mathcal{I}|$ linearly independent symmetric matrices.

As $0 \in \mathcal{F}(\mathcal{C}^*, X)$ and $\dim \mathcal{F}(\mathcal{C}^*, X) = m$, there must exist a set of linearly independent symmetric matrices $\{A_1, \dots, A_m\} \subseteq \mathcal{F}(\mathcal{C}^*, X)$. We have that $\langle A_j, X\rangle = 0$ for all j.

For all $i \in \mathcal{I}$, for all $j = 1, \dots, m$ and for all $\delta \in (0, 1)$, we have $A_j \in \mathcal{C}^*$ and $D_{\pm\delta,i} X D_{\pm\delta,i} \in \mathcal{C}$ and therefore, by the definition of the dual,

$$0 \leqslant \frac{1}{\delta}\langle A_j, D_{\pm\delta,i} X D_{\pm\delta,i}\rangle = \pm\langle A_j, \widetilde{X}_i\rangle + \delta\langle A_j, \widehat{X}_i\rangle.$$

Letting $\delta \to 0$ we get that $\langle A_j, \widetilde{X}_i\rangle = 0$ for all $i \in \mathcal{I}$, $j = 1, \dots, m$.

Therefore $\{\widetilde{X}_i \mid i \in \mathcal{I}\} \cup \{A_1, \dots, A_m\}$ is a set of linearly independent symmetric matrices, and this implies that $|\mathcal{I}| + m \leqslant \dim \mathcal{S}^n = \frac{1}{2}n(n+1)$. □

Using this lemma, we will now consider the maximal face given by a matrix $M \in \operatorname{Ext}(\mathcal{C}^n)$ such that $(M)_{ij} = \pm 1$ for all i, j, for example the Horn matrix, which was shown in [17] to give a face of dimension 10.

Theorem 6.5. *Let $M \in \operatorname{Ext}(\mathcal{C}^n)$ such that $(M)_{ij} = \pm 1$ for all i, j. Then $\mathcal{F}(\mathcal{C}^*, M)$ is a maximal face of $\mathcal{C}^{*n}$ with dimension $\frac{1}{2}n(n-1)$.*

Proof. From Theorems 2.20 and 4.6 it can be immediately seen that $\mathcal{F}(\mathcal{C}^*, M)$ is a maximal face of $\mathcal{C}^{*n}$.

As M is copositive we must have that $(M)_{ii} = 1$ for all i, and thus from Lemma 6.4 we have an upper bound of $\frac{1}{2}n(n-1)$ on the dimension of the face.

As in the proof of Theorem 4.6(iii) we now define the sets $\mathcal{J}_\pm$ and $\mathcal{J}_-$, along with a further set $\mathcal{J}_+$,

$$\mathcal{J}_- := \{(i,j) \mid i<j,\ (M)_{ij} = -1\},$$
$$\mathcal{J}_+ := \{(i,j) \mid i<j,\ (M)_{ij} = +1\},$$
$$\mathcal{J}_\pm := \{(i,j,k) \mid i<k,\ (M)_{ik} = -(M)_{ij} = -(M)_{jk} = 1\}.$$

We have that $\mathcal{J}_- \cup \mathcal{J}_+ = \{(i,j) \mid i<j,\ i,j = 1,\dots,n\}$ and $\mathcal{J}_- \cap \mathcal{J}_+ = \emptyset$.

As $M \in \operatorname{Ext}(\mathcal{C})$, from [13] we must have that $\mathcal{J}_+ = \{(i,k) \mid (i,j,k) \in \mathcal{J}_\pm\}$.

We now let $\widetilde{\mathcal{J}}_\pm$ be a minimal subset of $\mathcal{J}_\pm$ such that we maintain the property that $\mathcal{J}_+ = \{(i,k) \mid (i,j,k) \in \widetilde{\mathcal{J}}_\pm\}$. We then have that $|\widetilde{\mathcal{J}}_\pm| = |\mathcal{J}_+|$. We will now define $\mathcal{Y}_-$ as in the proof of Theorem 4.6(iii), along with a further two sets,

$$\mathcal{Y}_- := \{e_i + e_j \mid (i,j) \in \mathcal{J}_-\},$$
$$\widetilde{\mathcal{Y}}_\pm := \{e_i + 2e_j + e_k \mid (i,j,k) \in \widetilde{\mathcal{J}}_\pm\},$$
$$\mathcal{W} := \{vv^\mathsf{T} \mid v \in \mathcal{Y}_- \cup \widetilde{\mathcal{Y}}_\pm\}.$$

It is not difficult to show that $\mathcal{W} \subseteq \mathcal{F}(\mathcal{C}^{*n}, M)$ and $|\mathcal{W}| = \frac{1}{2}n(n-1)$. We will now show that $\mathcal{W}$ is a linearly independent set, which gives us a lower bound of $\frac{1}{2}n(n-1)$ on the dimension of the face and thus completes the proof.

Suppose by contradiction that $\mathcal{W}$ is not a linearly independent set. Then there must exist an $\alpha \in \mathcal{S}^n \setminus \{0\}$ such that $(\alpha)_{ii} = 0$ for all i and

$$M(\alpha) = 0, \quad \text{where we define}$$
$$M(\alpha) := \sum_{(i,j)\in\mathcal{J}_-} (\alpha)_{ij}(e_i+e_j)(e_i+e_j)^\mathsf{T}, + \sum_{(i,j,k)\in\widetilde{\mathcal{J}}_\pm} (\alpha)_{ik}(e_i+2e_j+e_k)(e_i+2e_j+e_k)^\mathsf{T}.$$

For an arbitrary $(i,k) \in \mathcal{J}_+$ we have that $0 = (M(\alpha))_{ik} = (\alpha)_{ik}$, and therefore $(\alpha)_{ik} = 0$ for all $(i,k) \in \mathcal{J}_+$. We now consider an arbitrary $(i,j) \in \mathcal{J}_-$, for which we have that $0 = (M(\alpha))_{i,j} = (\alpha)_{ij}$, and therefore $(\alpha)_{ij} = 0$ for all $(i,j) \in \mathcal{J}_-$ and so we have the contradiction that $(\alpha)_{ij} = 0$ for all i, j. $\square$

We finish this section by considering the maximal faces of the completely positive cone given by the matrices $e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}$, where $i \neq j$. We will show that these are in fact facets, as defined in Definition 2.1.

Theorem 6.6. *For $n \geqslant 2$ the completely positive cone $\mathcal{C}^{*n}$ has $\frac{1}{2}n(n-1)$ facets and they are of the following form,*

$$\mathcal{F}(\mathcal{C}^{*n}, e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}) = \{B \in \mathcal{C}^{*n} \mid (B)_{ij} = 0\} \quad \text{for } i<j,\ i,j = 1,\dots,n$$
$$= \left\{ \sum_k c_kc_k^\mathsf{T} \;\middle|\; c_k \in \mathbb{R}^n_+,\ (c_k)_i(c_k)_j = 0 \text{ for all } k \right\}.$$

Proof. From Theorem 2.17 any maximal face of the completely positive cone can be given by an extreme ray of the copositive cone, so we need only consider the faces $\mathcal{F}(\mathcal{C}^{*n}, X)$ where $X \in \operatorname{Ext}(\mathcal{C}^n)$. It has been shown in [14] that

$$\operatorname{Ext}(\mathcal{C}^n) \cap \mathcal{N}^n = \{\alpha(e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}) \mid \alpha > 0,\ i,j = 1,\dots,n\}.$$

We start this proof by considering the faces given by the vectors $e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}$ where $i<j$, proving them to be facets. We then consider the faces given by the vectors $e_ie_i^\mathsf{T}$, proving them not to be facets. As multiplying a vector by a strictly positive constant does not change the face it describes, the remaining faces to consider are given by matrices in $\operatorname{Ext}(\mathcal{C}^n) \setminus \mathcal{N}^n$, which we will prove are also not facets, completing the proof. For simplicity of notation in the proof, we let $N = \dim(\mathcal{C}^{*n}) = \dim(\mathcal{S}^n) = \frac{1}{2}n(n+1)$.

(i) Consider an arbitrary $i, j \in \{1,\dots,n\}$ such that $i<j$.

$(e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}) \in \mathcal{C}^n$, therefore (by Theorem 2.15) $\mathcal{F}(\mathcal{C}^{*n}, e_ie_j^\mathsf{T} + e_je_i^\mathsf{T})$ is an exposed face of $\mathcal{C}^{*n}$.

$$\mathcal{F}(\mathcal{C}^{*n}, e_ie_j^\mathsf{T} + e_je_i^\mathsf{T}) = \{B \in \mathcal{C}^{*n} \mid (B)_{ij} = 0\}$$
$$= \left\{ \sum_k c_kc_k^\mathsf{T} \;\middle|\; c_k \in \mathbb{R}^n_+,\ (c_k)_i(c_k)_j = 0 \text{ for all } k \right\}.$$

We now consider the set $\mathcal{Y}_{i,j}$ as defined in the proof of Theorem 4.6(i),

$$\mathcal{Y}_{i,j} := \{e_k + e_l \mid k \leqslant l,\ \{k,l\} \neq \{i,j\}\} \subset \mathbb{R}^n_+.$$

We have that $\{vv^\mathsf{T} \mid v \in \mathcal{Y}_{i,j}\} \subseteq \mathcal{F}(\mathcal{C}^{*n}, e_ie_j^\mathsf{T} + e_je_i^\mathsf{T})$.

Using Lemma 6.2 we see that the set $\{vv^{\mathsf{T}} \mid v \in \mathcal{Y}_{i,j}\}$ consists of $N-1$ linearly independent matrices. We also have that $0 \in \mathcal{F}(\mathcal{C}^{*n}, e_i e_j^{\mathsf{T}} + e_j e_i^{\mathsf{T}})$.

Therefore $N-1 \leqslant \dim \mathcal{F}(\mathcal{C}^{*n}, e_i e_j^{\mathsf{T}} + e_j e_i^{\mathsf{T}}) < \dim \mathcal{C}^{*n} = N$, and this implies that

$$\dim \mathcal{F}\big(\mathcal{C}^{*n}, e_i e_j^{\mathsf{T}} + e_j e_i^{\mathsf{T}}\big) = N-1 = \dim \mathcal{C}^{*n} - 1.$$

(ii) We shall now consider the faces given by $e_i e_i^{\mathsf{T}}$.

$$\begin{aligned}\mathcal{F}\big(\mathcal{C}^{*n}, e_i e_i^{\mathsf{T}}\big) &= \big\{B \in \mathcal{C}^{*n} \bigm| (B)_{ii} = 0\big\} \\ &= \left\{ \sum_k c_k c_k^{\mathsf{T}} \Bigm| c_k \in \mathbb{R}^n_+,\ (c_k)_i = 0 \text{ for all } k \right\} \\ &= \big\{B \in \mathcal{C}^{*n} \bigm| (B)_{ij} = 0 \text{ for all } j\big\} \\ &\subset \mathcal{F}\big(\mathcal{C}^{*n}, e_i e_j^{\mathsf{T}} + e_j e_i^{\mathsf{T}}\big) \quad \text{for all } j \neq i.\end{aligned}$$

Therefore these faces cannot be facets.

(iii) Now it is only left for us to consider the faces given by the matrices in $\operatorname{Ext}(\mathcal{C}^n) \setminus \mathcal{N}^n$. For an arbitrary matrix $X \in \operatorname{Ext}(\mathcal{C}^n) \setminus \mathcal{N}^n$ there must exist an i, j such that $(X)_{ij} < 0$ and from Theorem 1.1 we must have that $i \neq j$ and $(X)_{ii}, (X)_{jj} > 0$. We can now use Lemma 6.4 to show that $\dim(\mathcal{F}(\mathcal{C}^{*n}, X)) \leqslant \dim \mathcal{C}^{*n} - 2$. $\square$

7. Lower bound on the dimension of maximal faces of the completely positive cone

In all of our examples of maximal faces of the completely positive cone so far looked at we have had that their dimensions were greater than or equal to $\frac{1}{2}n(n-1)$. From this one might suspect that this is in fact a lower bound on the dimension of the maximal faces for the completely positive cone, as it was for the copositive cone. For $n \leqslant 4$ we know all the extreme rays of the copositive cone and from the analysis in the previous section we see that the conjecture does hold in this case. We will however show that the conjecture is not generally true by giving an example of a copositive matrix which gives an exposed ray of the copositive cone, implying that it also gives a maximal face of the completely positive cone, however the dimension of this face is strictly less than the conjectured lower bound.

Before we can do this we need to know how we can take a known copositive matrix, check if it gives an exposed ray and find the dimension of the exposed face given by it. In order to do this we first introduce the concept of the set of zeros in the nonnegative orthant for a quadratic form, as used previously in [18]. This is defined as follows for a matrix $B \in \mathcal{S}^n$,

$$\mathcal{V}^B := \big\{v \in \mathbb{R}^n_+ \bigm| v^{\mathsf{T}} B v = 0\big\}.$$

The theorems below give two of the properties of this set.

Theorem 7.1. *Suppose the matrix $\widehat{A} \in \mathcal{C}^n$ and the vector $\hat{x} \in \mathbb{R}^n_+$ can be partitioned as below, where $p \leqslant n$, $A \in \mathcal{S}^p$, $B \in \mathbb{R}^{p\times(n-p)}$, $C \in \mathcal{S}^{n-p}$ and $x \in \mathbb{R}^p_{++}$.*

$$\widehat{A} = \begin{pmatrix} A & B \\ B^{\mathsf{T}} & C \end{pmatrix}, \qquad \hat{x} = \begin{pmatrix} x \\ 0 \end{pmatrix}.$$

Then we have that $\hat{x} \in \mathcal{V}^{\widehat{A}}$ if and only if A is a positive semidefinite matrix and $x \in \operatorname{Ker}(A)$, where $\operatorname{Ker}(A)$ denotes the kernel of A.

Proof. We have that $\hat{x}^{\mathsf{T}}\widehat{A}\hat{x} = x^{\mathsf{T}}Ax$. From this the reverse implication is trivial. To prove the forward implication we first suppose that $\hat{x}^{\mathsf{T}}\widehat{A}\hat{x} = 0$. This implies that $x^{\mathsf{T}}Ax = 0$. From Theorem 1.1 this in turn implies that A is positive semidefinite and from the properties of positive semidefinite matrices we also get that $Ax = 0$. $\square$

Theorem 7.2. *Suppose the matrix $\widehat{A} \in \mathcal{C}^n$ and the vector $\hat{x} \in \mathbb{R}^n$ can be partitioned as below, where $p \leqslant n$, $A \in \mathcal{S}^p_+$, $B \in \mathbb{R}^{p\times(n-p)}$, $C \in \mathcal{S}^{n-p}$ and $x \in \mathbb{R}^p$.*

$$\widehat{A} = \begin{pmatrix} A & B \\ B^{\mathsf{T}} & C \end{pmatrix}, \qquad \hat{x} = \begin{pmatrix} x \\ 0 \end{pmatrix}.$$

Then we have that $\hat{x} \in \mathcal{V}^{\widehat{A}}$ if and only if $x \in \mathbb{R}^p_+ \cap \operatorname{Ker}(A)$.

Proof. $\hat{x}^{\mathsf{T}}\widehat{A}\hat{x} = 0 \Leftrightarrow x^{\mathsf{T}}Ax = 0 \Leftrightarrow Ax = 0$. $\square$

From these properties we immediately get the following two techniques.

Method 7.3. Theorems 7.1 and 7.2 can be easily extended by considering permutations of the coordinate basis. From this we see that for a given copositive matrix A we can find $\mathcal{V}^A$ by first finding the maximal positive semidefinite principal submatrices of A and then considering their kernels. Applying this method for a given copositive matrix A we find its set of zeros in the nonnegative orthant in the form

$$\mathcal{V}^A = \bigcup_{i=1}^{m} \operatorname{cone} \mathcal{X}_i,$$

where $\mathcal{X}_i \subset \mathbb{R}^n_+$ is a finite set for all i and where we define a conic hull of a set $\mathcal{Q}$ as follows,

$$\operatorname{cone} \mathcal{Q} := \left\{ \sum_i \theta_i q_i \;\middle|\; \theta_i \geqslant 0,\ q_i \in \mathcal{Q} \text{ for all } i \right\}.$$

Each $\mathcal{X}_i$ relates to the set of exposed rays from the intersection of the nonnegative orthant with the kernel of a maximal positive semidefinite principal submatrix.

Method 7.4. We can also partially reverse the process in the previous method. Given a finite set $\mathcal{V} \subset \mathbb{R}^n_+$ we can find necessary conditions on a matrix $A \in \mathcal{C}$ in order to have $\mathcal{V} \subset \mathcal{V}^A$. These necessary conditions are in terms of certain principal submatrices being positive semidefinite and containing certain vectors in their kernels.

We now present the following theorem which gives an application of these methods.

Theorem 7.5. *Consider a matrix $A \in \mathcal{C} \setminus \{0\}$. Let $\{\mathcal{X}_1, \dots, \mathcal{X}_m\}$ be such that $\mathcal{X}_i \subset \mathbb{R}^n_+$ is a finite set for all i and*

$$\mathcal{V}^A = \bigcup_{i=1}^{m} \operatorname{cone} \mathcal{X}_i.$$

Using Method 7.3 we can always find such a set. We now define the following for $i = 1, \dots, m$:

$$\mathcal{Y}_i = \{b_1 + b_2 \mid b_1, b_2 \in \mathcal{X}_i\},$$
$$\mathcal{Z}_i = \{bb^\mathsf{T} \mid b \in \mathcal{Y}_i\} = \{(b_1 + b_2)(b_1 + b_2)^\mathsf{T} \mid b_1, b_2 \in \mathcal{X}_i\}.$$

Then we have that:

(i) $\operatorname{cone}(\bigcup_{i=1}^m \mathcal{Z}_i) \subseteq \mathcal{F}(\mathcal{C}^*, A) \subseteq \operatorname{span}(\bigcup_{i=1}^m \mathcal{Z}_i)$, *where we define the linear span of a set $\mathcal{Q}$ as follows,*

$$\operatorname{span} \mathcal{Q} := \left\{ \sum_i \theta_i q_i \;\middle|\; \theta_i \in \mathbb{R},\ q_i \in \mathcal{Q} \text{ for all } i \right\}.$$

(ii) $\dim \mathcal{F}(\mathcal{C}^*, A) = \dim(\operatorname{span}(\bigcup_{i=1}^m \mathcal{Z}_i))$. *(Note that as $\mathcal{Z}_i$ is a finite set this value is relatively easy to compute.)*

(iii) $A \in \operatorname{Exp}(\mathcal{C}) \Leftrightarrow \{X \in \mathcal{C} \mid \bigcup_{i=1}^m \mathcal{Y}_i \subseteq \mathcal{V}^X\} = \{\alpha A \mid \alpha \geqslant 0\}$.

Proof. We begin by noting the following, where $\mathcal{B} \subset \mathbb{R}^n_+$ is a finite set,

$$\mathcal{F}(\mathcal{C}^*, A) = \left\{ \sum_i b_i b_i^\mathsf{T} \;\middle|\; b_i \in \mathbb{R}^n_+ \text{ for all } i,\ \sum_i b_i^\mathsf{T} A b_i = 0 \right\} = \operatorname{cone}\{bb^\mathsf{T} \mid b \in \mathcal{V}^A\},$$

$$\mathcal{F}\left(\mathcal{C}, \sum_{b \in \mathcal{B}} bb^\mathsf{T}\right) = \left\{ X \in \mathcal{C} \;\middle|\; \sum_{b \in \mathcal{B}} b^\mathsf{T} X b = 0 \right\} = \{X \in \mathcal{C} \mid \mathcal{B} \subset \mathcal{V}^X\}.$$

We now prove each point in turn.

(i) We have that

$$\operatorname{cone}\left(\bigcup_{i=1}^{m} \mathcal{Z}_i\right) \subseteq \operatorname{cone}\{bb^\mathsf{T} \mid b \in \mathcal{V}^A\} = \mathcal{F}(\mathcal{C}^*, A).$$

We also have that

$$\begin{aligned}
\mathcal{F}(\mathcal{C}^*, A) &= \operatorname{cone}\{bb^\mathsf{T} \mid b \in \mathcal{V}^A\} \\
&\subseteq \operatorname{span} \bigcup_{i=1}^m \{bb^\mathsf{T} \mid b \in \operatorname{cone} \mathcal{X}_i\} \\
&= \operatorname{span} \bigcup_{i=1}^m \left\{ \left(\sum_j \alpha_j b_j\right)\left(\sum_k \alpha_k b_k\right)^\mathsf{T} \,\middle|\, \alpha_l \geqslant 0,\ b_l \in \mathcal{X}_i \text{ for all } l \right\} \\
&= \operatorname{span} \bigcup_{i=1}^m \left\{ \frac{1}{2} \sum_{j,k} \alpha_j \alpha_k \left(b_j b_k^\mathsf{T} + b_k b_j^\mathsf{T}\right) \,\middle|\, \alpha_l \geqslant 0,\ b_l \in \mathcal{X}_i \text{ for all } l \right\} \\
&= \operatorname{span} \bigcup_{i=1}^m \left\{ \frac{1}{8} \sum_{j,k} \alpha_j \alpha_k \left(4(b_j + b_k)(b_j + b_k)^\mathsf{T} - (b_j + b_j)(b_j + b_j)^\mathsf{T} \right.\right. \\
&\qquad \left.\left. - (b_k + b_k)(b_k + b_k)^\mathsf{T}\right) \,\middle|\, \alpha_l \geqslant 0,\ b_l \in \mathcal{X}_i \text{ for all } l \right\} \\
&\subseteq \operatorname{span}\left(\bigcup_{i=1}^m (\operatorname{span} \mathcal{Z}_i) \right) = \operatorname{span}\left(\bigcup_{i=1}^m \mathcal{Z}_i \right).
\end{aligned}$$

(ii) This is implied directly from part (i).

(iii) From part (i) we see that $\sum_{i=1}^m \sum_{b \in \mathcal{Y}_i} bb^\mathsf{T} \in \operatorname{reint}(\mathcal{F}(\mathcal{C}^*, A))$. From Theorem 2.21 we have that the minimal exposed face of the copositive cone containing A is given by

$$\mathcal{F}\left(\mathcal{C}, \sum_{i=1}^m \sum_{b \in \mathcal{Y}_i} bb^\mathsf{T}\right) = \left\{ X \in \mathcal{C}^n \,\middle|\, \bigcup_{i=1}^m \mathcal{Y}_i \subseteq \mathcal{V}^X \right\}.$$

We now note that A gives an exposed ray if and only if the minimal exposed face containing it is a ray. □

We now present our counter example to the conjectured lower bound.

Theorem 7.6. *If we let A be the matrix given below then we have that $\mathcal{F}(\mathcal{C}^*, A)$ is a maximal face of the completely positive cone and $\dim \mathcal{F}(\mathcal{C}^*, A) = 27$, which is strictly less than the conjectured lower bound, $\frac{1}{2}(9)(9-1) = 36$.*

$$A = \begin{pmatrix}
1 & -1 & 1 & 0 & 0 & 0 & 0 & 1 & -1 \\
-1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & 1 \\
1 & -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -1 & 1 & -1 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 1 & -1 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 \\
1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\
-1 & 1 & 0 & 0 & 0 & 0 & 1 & -1 & 1
\end{pmatrix}.$$

(*This matrix is referred to as a Hoffman–Pereira matrix.*)

Proof. From [13] we have that $A \in \operatorname{Ext}(\mathcal{C})$. Using Method 7.3 we find $\mathcal{V}^A$, which is given as follows.

$$\mathcal{V}^A = \bigcup_{\substack{\text{Cyclic} \\ \text{Permutations}}} \operatorname{cone}\left\{ \begin{pmatrix} 1\\1\\0\\0\\0\\0\\0\\0\\0 \end{pmatrix}, \begin{pmatrix} 0\\1\\1\\0\\0\\0\\0\\0\\0 \end{pmatrix}, \begin{pmatrix} 0\\0\\0\\0\\0\\1\\1\\0\\0 \end{pmatrix} \right\}.$$

Now using Theorem 7.5(iii) and Method 7.4 we get that $A \in \operatorname{Exp}(\mathcal{C})$, therefore from Theorem 2.20 we see that $\mathcal{F}(\mathcal{C}^*, A)$ is a maximal face of the copositive cone. Using Theorem 7.5(ii) we have that $\dim \mathcal{F}(\mathcal{C}^*, A) = 27$. □

Finding the actual value of the tight lower bound for the dimension of a maximal face of the completely positive cone is still an open question. The methods in this section can be used to test specific examples of copositive matrices, however we would run in to problems if given a copositive matrix which did not lie on an exposed ray and, unbeknown to us, gave a maximal face of the completely positive cone. We do not currently have any examples of a matrix like this and it is another open question as to whether such a matrix does in fact exist.

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