The extreme rays of the 6 x 6 copositive cone

Andrey Afonin, Roland Hildebrand, Peter J. C. Dickinson

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Abstract

We provide a complete classification of the extreme rays of the 6×6 copositive cone $\mathcal{COP}^6$. We proceed via a coarse intermediate classification of the possible minimal zero support set of an exceptional extremal matrix $A \in \mathcal{COP}^6$. To each such minimal zero support set we construct a stratified semi-algebraic manifold in the space of real symmetric 6×6 matrices $\mathcal{S}^6$, parameterized in a semi-trigonometric way, which consists of all exceptional extremal matrices $A \in \mathcal{COP}^6$ having this minimal zero support set. Each semi-algebraic stratum is characterized by the supports of the minimal zeros u as well as the supports of the corresponding matrix-vector products Au. The analysis uses recently and newly developed methods that are applicable also to copositive matrices of arbitrary order.

Keywords: copositive matrix, extreme ray, minimal zero, non-convex optimization

1 Introduction

An element A of the space $\mathcal{S}^n$ of real symmetric $n \times n$ matrices is called *copositive* if $x^T Ax \geq 0$ for all vectors $x \in \mathbb{R}^n_+$. The set of such matrices forms the *copositive cone* $\mathcal{COP}^n$. This cone plays an important role in non-convex optimization, as many difficult optimization problems can be reformulated as conic programs over $\mathcal{COP}^n$. For a detailed survey of the applications of this cone see, e.g., [13, 2, 3, 19].

Verifying copositivity of a given matrix is a co-NP-complete problem [21], and the complexity of the copositive cone quickly grows with dimension. It is a classical result by Diananda [6, Theorem 2] that for $n \leq 4$ the copositive cone can be described as the sum of the cone of positive semi-definite matrices $\mathcal{S}^n_+$ and the cone of element-wise nonnegative symmetric matrices $\mathcal{N}^n$. In general, this sum is a subset of the copositive cone, $\mathcal{S}^n_+ + \mathcal{N}^n \subset \mathcal{COP}^n$. Matrices in the difference $\mathcal{COP}^n \setminus (\mathcal{S}^n_+ + \mathcal{N}^n)$ are called *exceptional*.

In this note we focus on the extreme rays of $\mathcal{COP}^n$. A non-zero matrix $A \in \mathcal{COP}^n$ is called *extremal* if a decomposition $A = A_1 + A_2$ of A into matrices $A_1, A_2 \in \mathcal{COP}^n$ is only possible if $A_1 = \lambda A$, $A_2 = (1-\lambda)A$ for some $\lambda \in [0, 1]$. The set of positive multiples of an extremal matrix is called an *extreme ray* of $\mathcal{COP}^n$. The set of extreme rays is an important characteristic of a convex cone. Its structure, first of all its stratification into a union of manifolds of different dimension, yields much information about the shape of the cone. The extreme rays of a convex cone which is algorithmically difficult to access are especially important if one wishes to check the tightness of inner convex approximations of the cone. Namely, an inner approximation is exact if and only if it contains all extreme rays, see [11] for such a construction applied to the cone $\mathcal{COP}^5$.

Since the extreme rays of a cone determine the facets of its dual cone, they are also important tools for the study of this dual cone. The extreme rays of the copositive cone have been used in a number of papers on its dual, the completely positive cone [7, 24, 4, 5, 23, 22].

There are few results on the extreme rays of $\mathcal{COP}^n$. The non-exceptional extreme rays of $\mathcal{COP}^n$ have been classified in [14]. The exceptional extreme rays of $\mathcal{COP}^5$ have been described in [16]. In [1, Theorem 3.8] a procedure is presented how to construct an extreme ray of $\mathcal{COP}^{n+1}$ from an extreme ray of $\mathcal{COP}^n$. Those extreme rays of $\mathcal{COP}^n$ with elements only from the set $\{-1, 0, +1\}$ have been characterized in [20]. In [18, 9] large families of extreme rays of $\mathcal{COP}^n$ have been constructed. In [8] a family of extreme rays of $\mathcal{COP}^6$ has been constructed. In this paper we complete the classification the extreme rays of $\mathcal{COP}^6$.

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A useful tool in the study of extremal copositive matrices are its zeros [6, 1]. A *zero* u of a copositive matrix A is a non-zero nonnegative vector such that $u^T Au = 0$. The *support* $\operatorname{supp} u$ of a zero $u = (u_1, \ldots, u_n)^T \in \mathbb{R}^n_+$ is the subset of indices $j \in \{1, \ldots, n\}$ such that $u_j > 0$. A zero u of A is called *minimal* if there is no zero v of A such that $\operatorname{supp} v \subset \operatorname{supp} u$ holds strictly. The *minimal zero support set*, i.e., the ensemble $\operatorname{supp} \mathcal{V}^A_{\min}$ of minimal zero supports of a copositive matrix A is an informative characteristic of the matrix [17]. It is a subset of $2^{\{1,\ldots,n\}}$, the power set of $\{1, \ldots, n\}$. We shall use this combinatorial characteristic to achieve the classification of the extreme rays of $\mathcal{COP}^6$.

In [17, Table 1] the list of possible minimal zero support sets of an exceptional extremal matrix $A \in \mathcal{COP}^6$ with positive diagonal has been narrowed down to 44 index sets, up to a permutation of the indices. In Table 1 we reproduce this list up to permutations of the index set $\{1, \ldots, 6\}$. We consider each of these index sets and determine whether it can actually be a minimal zero support set of an exceptional extremal matrix $A \in \mathcal{COP}^6$. We find that in 19 out of the 44 cases the answer to this question is affirmative, and for each of the corresponding index sets we determine all exceptional extremal matrices $A \in \mathcal{COP}^6$ which have the given index set as its minimal zero support set. For convenience the cases have been assigned new numbers, which are given in Table 1 along with the numbers from [17]. In the last column of Table 1 we summarize our findings on the different cases.

The remainder of the paper is structured as follows. In Section 2 we consider the non-exceptional extreme rays of $\mathcal{COP}^6$ and those which can be obtained by padding the extremal matrices of $\mathcal{COP}^5$ with zeros. In Section 3 we present a general strategy of how to determine all exceptional extremal matrices $A \in \mathcal{COP}^6$ which have a given minimal zero support set $\mathcal{I} \subset 2^{\{1,\ldots,6\}}$. If there are such matrices, we shall describe them explicitly by parameterizing the set of these matrices by a finite number of variables varying in some domain, thus assigning to the index set $\mathcal{I}$ one or several submanifolds $M_{\mathcal{I}} \subset \mathcal{S}^6$ of extremal exceptional copositive matrices. These manifolds are described in Section 5, along with Theorem 5.1 formalizing the classification of the extreme rays of the cone $\mathcal{COP}^6$. The strategy presented in Section 3 achieves its goal for most of the index sets in Table 1. The few remaining cases necessitate an individual approach, which will be presented in Section 4. Finally, we summarize our finding in Section 6, where we also consider perspectives for future work.

1.1 Notations

The space of real symmetric matrices of size $n \times n$ will be denoted by $\mathcal{S}^n$. The cone of positive semi-definite matrices in $\mathcal{S}^n$ will be denoted by $\mathcal{S}^n_+$, and the cone of element-wise nonnegative matrices by $\mathcal{N}^n$.

We shall denote vectors with lower-case letters and matrices with upper-case letters. Individual entries of a vector u and a matrix A will be denoted by u_i and A_{ij} respectively. For a matrix A and a vector u of compatible dimension, the i-th element of the matrix-vector product Au will be denoted by $(Au)_i$. Inequalities $u \geq \mathbf{0}$ on vectors will be meant element-wise, where we denote by $\mathbf{0} = (0, \ldots, 0)^T$ the all-zeros vector. Similarly we denote by $\mathbf{1} = (1, \ldots, 1)^T$ the all-ones vector. We further let e_i be the unit vector with i-th entry equal to one and all other entries equal to zero. For a subset $I \subset \{1, \ldots, n\}$ we denote by A_I the principal submatrix of A whose elements have row and column indices in I, i.e. $A_I = (A_{ij})_{i,j \in I} \in \mathcal{S}^{|I|}$. Similarly for a vector $u \in \mathbb{R}^n$ we define the subvector $u_I = (u_i)_{i \in I} \in \mathbb{R}^{|I|}$. By E_{ij} we denote a matrix which has all entries equal to zero except (i, j) and (j, i), which equal 1.

Let $\mathcal{I} \subset 2^{\{1,\ldots,n\}}$ be an index set. We say that an element A_{ij} of $A \in \mathcal{S}^n$ is *covered* by $\mathcal{I}$ if there exists $I \in \mathcal{I}$ such that $i, j \in I$.

We call a vector $u \in \mathbb{R}^n_+ \setminus \{\mathbf{0}\}$ a *zero* of a matrix $A \in \mathcal{COP}^n$ if $u^T Au = 0$, and we denote the set of zeros of A by $\mathcal{V}^A = \{u \mid u^T Au = 0\}$. For a vector $u \in \mathbb{R}^n$ we define its *support* as $\operatorname{supp} u = \{i \in \{1, \ldots, n\} \mid u_i \neq 0\}$. We also define $\operatorname{supp}_+ u = \{i \in \{1, \ldots, n\} \mid u_i > 0\}$ and $\operatorname{supp}_{\geq 0} u = \{i \in \{1, \ldots, n\} \mid u_i \geq 0\}$. Note that for zeros of copositive matrices the two notions $\operatorname{supp}_+ u$ and $\operatorname{supp} u$ are equivalent.

A zero u of a copositive matrix A is called *minimal* if there exists no zero v of A such that the inclusion $\operatorname{supp} v \subset \operatorname{supp} u$ holds strictly. We shall denote the set of minimal zeros of a copositive matrix A by $\mathcal{V}^A_{\min}$ and the ensemble of supports of the minimal zeros of A by $\operatorname{supp} \mathcal{V}^A_{\min}$.

Finally, let us introduce the following notion. A copositive matrix A is called *irreducible* with respect to another copositive matrix C if for every $\delta > 0$, we have $A - \delta C \notin \mathcal{COP}^n$, and it is called irreducible with respect to a subset $\mathcal{M} \subset \mathcal{COP}^n$ if it is irreducible with respect to all nonzero elements $C \in \mathcal{M}$.

2 Lower order and non-exceptional extreme rays

In this section we classify the extreme rays of $\mathcal{COP}^6$ which are not exceptional or which are effectively of order 5.

The former have been described in [14]. They are generated by the matrices E_{ij}, $1 \le i, j \le 6$, and by rank 1 matrices aa^T such that the vector a has positive as well as negative elements. Note that by multiplying the extremal matrix by a positive definite diagonal matrix from the left and from the right, we may achieve that the elements of a are in the set $\{-1, 0, +1\}$. By multiplying a by -1 we achieve that the number of positive elements is not smaller than the number of negative elements.

The exceptional extreme rays of $\mathcal{COP}^5$ have been described in [16]. They are generated by matrices of the form $P^T DADP$, where $P \in S_5$ is a permutation matrix, D is a positive diagonal matrix, and A is given by

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_5 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_5) \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) \\ \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 \\ -\cos\phi_5 & \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 \end{pmatrix},$$

where either $\phi_1 = \cdots = \phi_5 = 0$, or $\phi_i > 0$ for $i = 1, \ldots, 5$ and $\sum_{i=1}^5 \phi_i < \pi$. By adding a zero column and a zero row to an extremal matrix of $\mathcal{COP}^5$ we obtain an extremal matrix of $\mathcal{COP}^6$.

All other non-zero extremal matrices of $\mathcal{COP}^6$ are exceptional and have positive diagonal elements. They will be considered in the following two sections.

3 General algorithm

Out of the 44 index sets in Table 1 there are two (cases 19 and 41) which contain supports of cardinality 4 and require a separate consideration. All other index sets contain only supports of cardinality 2 and 3, and can be treated by a common general scheme. This scheme will be described in this section. Due to space limitations we shall not give a full proof in each case, but rather describe the method, which is the same for all cases, and furnish intermediate results in the form of tables. A detailed treatment of the most complicated case No. 19 is provided in Section 4, the calculations for the cases in this section are similar.

3.1 Parametrization

Our goal is to find all exceptional extremal copositive matrices A with a given set $\mathcal{I} \subset 2^{\{1,\ldots,6\}}$ of minimal zero supports. Every index set from $\mathcal{I}$ imposes conditions on the matrix A by virtue of the presence of the corresponding minimal zero. Therefore $\mathcal{I}$ determines a submanifold $M_{\mathcal{I}}$ of candidate extremal copositive matrices $A \in \mathcal{S}^6$ with minimal zero support set $\mathcal{I}$. In this section we describe our method of parameterizing $A \in M_{\mathcal{I}}$ and its minimal zeros in a convenient manner. Equivalently, we construct a coordinate chart on the manifold $M_{\mathcal{I}}$.

Let us first consider the diagonal elements of the copositive matrix A, which can be either positive or zero. If one or more of the diagonal elements of an exceptional extremal copositive matrix A are zero, then A equals an extremal copositive matrix of strictly lower order, padded with zeros. These have been already considered in Section 2. We shall hence assume that all diagonal elements of A are positive. By the transformation $A \mapsto DAD$, where D is a diagonal matrix with positive diagonal elements, the diagonal elements of A can be normalized to 1. This transformation preserves the copositive cone as well as the minimal zero support set of A. We shall hence assume that $A_{ii} = 1$ for $i = 1, \ldots, 6$. A general exceptional extremal matrix $A \in \mathcal{COP}^6$ with minimal zero support set $\mathcal{I}$ can be obtained from the normalized matrices by scaling with arbitrary positive definite diagonal matrices D.

We are left with 15 off-diagonal elements A_{ij}, $1 \le i < j \le 6$, to determine. By a result of Hall and Newman [14], we may assume that $A_{ij} \in [-1, 1]$ for all i, j. This allows us to represent the element A_{ij} as $-\cos\phi_{ij}$ with $\phi_{ij} \in [0, \pi]$.

Let us now provide some results which demonstrate the way a support of a minimal zero with cardinality 2 or 3 imposes conditions on the elements of the matrix A.

Lemma 3.1. *[10, Corollary 4.4] Let $A \in \mathcal{COP}^n$ with $A_{ii} = 1$ for all i, and let $u \in \mathcal{V}^A_{\min}$ with $\operatorname{supp} u = \{i, j\}$ for some indices $i, j \in \{1, \ldots, n\}$. Then $A_{ij} = -1$ and the two positive elements of u are equal.*

Extremal copositive matrices are irreducible with respect to the nonnegative cone $\mathcal{N}^n$ if they have more than one non-zero diagonal element. Hence the following result is a direct consequence of [10, Lemma 4.6].

Lemma 3.2. *Let $A \in \mathcal{COP}^n$ be extremal and $A_{ii} = 1$ for all i. Suppose $\{i, j\}, \{j, k\} \in \operatorname{supp} \mathcal{V}^A_{\min}$, where i, j, k are mutually different indices. Then $A_{\{i,j,k\}}$ is a rank 1 positive semi-definite matrix with $A_{ik} = -A_{ij} = -A_{jk} = 1$.*

The following result is a direct consequence of [17, Lemma 5.4 (e)] and [10, Lemma 4.7].

Lemma 3.3. *Let $A \in \mathcal{COP}^n$ have unit diagonal and suppose there exists a minimal zero u of A with support $\{i, j, k\}$, where $i, j, k \in \{1, \ldots, n\}$ are mutually different indices. Then the submatrix $A_{\{i,j,k\}}$ is given by*

$$\begin{pmatrix} 1 & -\cos\phi_k & -\cos\phi_j \\ -\cos\phi_k & 1 & -\cos\phi_i \\ -\cos\phi_j & -\cos\phi_i & 1 \end{pmatrix},$$

where $\phi_i, \phi_j, \phi_k \in (0, \pi)$ and $\phi_i + \phi_j + \phi_k = \pi$. Moreover, there exists $\lambda > 0$ such that $\lambda u_{\{i,j,k\}} = (\sin\phi_i, \sin\phi_j, \sin\phi_k)^T$.

These results allow us to parameterize some of the off-diagonal elements by a number of angles ϕ_i which vary in a certain open polytope. Note that there are relations on the angles of equality type which allow to eliminate some of them. However, in general this covers only a part of the off-diagonal entries of the matrix A, in particular, those which are covered by the index set $\mathcal{I}$. The remaining entries of A will be parameterized by variables $b_i \in [-1, 1]$. The construction guarantees that the matrix A indeed has minimal zeros with the given supports.

For the cases 1–19 of Table 1 the parametrizations are given in Section 5, with the location of the variables b_i in Table 2, if there are any such elements.

In case 14 of Table 1 the matrix A does not contain any parameters at all and is determined uniquely at this stage. It is exceptional extremal by the criterion of Haynsworth and Hoffman [15, Theorem 3.1].

For the cases 20–29 and 42 we obtain the following parametrizations, respectively:

$$20: \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & b_1 & b_2 \\ 1 & -1 & 1 & b_1 & 1 & -1 \\ 1 & 1 & -1 & b_2 & -1 & 1 \end{pmatrix},$$

$$21: \begin{pmatrix} 1 & -1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & -\cos\phi_4 \\ -1 & 1 & b_1 & b_2 & \cos(\phi_5+\phi_6) & -\cos\phi_6 \\ -\cos\phi_2 & b_1 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & \cos(\phi_3+\phi_5) \\ -\cos\phi_1 & b_2 & \cos(\phi_1+\phi_2) & 1 & b_3 & \cos(\phi_1+\phi_4) \\ \cos(\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_3 & b_3 & 1 & -\cos\phi_5 \\ -\cos\phi_4 & -\cos\phi_6 & \cos(\phi_3+\phi_5) & \cos(\phi_1+\phi_4) & -\cos\phi_5 & 1 \end{pmatrix},$$

$$22: \begin{pmatrix} 1 & -1 & b_1 & b_2 & b_3 & b_4 \\ -1 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_5 \\ b_1 & -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos(\phi_5+\phi_1) \\ b_2 & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) \\ b_3 & \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 \\ b_4 & -\cos\phi_5 & \cos(\phi_5+\phi_1) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 \end{pmatrix},$$

$$23: \begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & b_1 & b_2 \\ -1 & 1 & \cos(\phi_3+\phi_4) & \cos(\phi_5+\phi_6) & -\cos\phi_4 & -\cos\phi_6 \\ -\cos\phi_2 & \cos(\phi_3+\phi_4) & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_1+\phi_5) \\ \cos(\phi_1+\phi_2) & \cos(\phi_5+\phi_6) & -\cos\phi_1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_5 \\ b_1 & -\cos\phi_4 & -\cos\phi_3 & \cos(\phi_1+\phi_3) & 1 & b_3 \\ b_2 & -\cos\phi_6 & \cos(\phi_1+\phi_5) & -\cos\phi_5 & b_3 & 1 \end{pmatrix},$$

$$24:\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_4 & b_1 \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_5+\phi_6) & \cos(\phi_5+\phi_7) & -\cos\phi_5 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_5+\phi_6) & 1 & b_2 & -\cos\phi_6 \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & \cos(\phi_5+\phi_7) & b_2 & 1 & -\cos\phi_7 \\ \cos(\phi_1+\phi_5) & b_1 & -\cos\phi_5 & -\cos\phi_6 & -\cos\phi_7 & 1 \end{pmatrix},$$

$$25:\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_4 & b_1 \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_5+\phi_6) & b_2 & -\cos\phi_5 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_5+\phi_6) & 1 & \cos(\phi_6+\phi_7) & -\cos\phi_6 \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & b_2 & \cos(\phi_6+\phi_7) & 1 & -\cos\phi_7 \\ \cos(\phi_1+\phi_5) & b_1 & -\cos\phi_5 & -\cos\phi_6 & -\cos\phi_7 & 1 \end{pmatrix},$$

$$26:\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_4) & b_1 \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & \cos(\phi_3+\phi_5) & -\cos(\phi_1+\phi_2-\phi_6) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_4+\phi_5) & -\cos\phi_4 & -\cos\phi_6 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_4+\phi_5) & 1 & -\cos\phi_5 & b_2 \\ \cos(\phi_1+\phi_4) & \cos(\phi_3+\phi_5) & -\cos\phi_4 & -\cos\phi_5 & 1 & b_3 \\ b_1 & -\cos(\phi_1+\phi_2-\phi_6) & -\cos\phi_6 & b_2 & b_3 & 1 \end{pmatrix},$$

$$27:\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_4) & b_1 \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & \cos(\phi_3+\phi_5) & b_2 \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & -\cos\phi_7 & -\cos\phi_4 & -\cos\phi_6 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & -\cos\phi_7 & 1 & -\cos\phi_5 & \cos(\phi_6+\phi_7) \\ \cos(\phi_1+\phi_4) & \cos(\phi_3+\phi_5) & -\cos\phi_4 & -\cos\phi_5 & 1 & \cos(\phi_4+\phi_6) \\ b_1 & b_2 & -\cos\phi_6 & \cos(\phi_6+\phi_7) & \cos(\phi_4+\phi_6) & 1 \end{pmatrix},$$

$$28:\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & -\cos\phi_4 & \cos(\phi_4+\phi_6) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & \cos(\phi_3+\phi_5) & b_1 \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & b_2 & \cos(\phi_1+\phi_4) & b_3 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & b_2 & 1 & -\cos\phi_5 & \cos(\phi_5+\phi_6) \\ -\cos\phi_4 & \cos(\phi_3+\phi_5) & \cos(\phi_1+\phi_4) & -\cos\phi_5 & 1 & -\cos\phi_6 \\ \cos(\phi_4+\phi_6) & b_1 & b_3 & \cos(\phi_5+\phi_6) & -\cos\phi_6 & 1 \end{pmatrix},$$

$$29:\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & -\cos\phi_4 & \cos(\phi_4+\phi_6) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & b_1 & \cos(\phi_5+\phi_6) & -\cos\phi_5 \\ -\cos\phi_3 & \cos(\phi_2+\phi_3) & b_1 & 1 & b_2 & -\cos(\phi_1+\phi_5-\phi_3) \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & \cos(\phi_5+\phi_6) & b_2 & 1 & -\cos\phi_6 \\ \cos(\phi_1+\phi_5) & \cos(\phi_4+\phi_6) & -\cos\phi_5 & -\cos(\phi_1+\phi_5-\phi_3) & -\cos\phi_6 & 1 \end{pmatrix},$$

$$42:\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_4) & b_1 \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_5 & -\cos\phi_6 \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & b_2 & -\cos\phi_4 & -\cos(\phi_1+\phi_2-\phi_6) \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & b_2 & 1 & \cos(\phi_3+\phi_5) & b_3 \\ \cos(\phi_1+\phi_4) & -\cos\phi_5 & -\cos\phi_4 & \cos(\phi_3+\phi_5) & 1 & \cos(\phi_5+\phi_6) \\ b_1 & -\cos\phi_6 & -\cos(\phi_1+\phi_2-\phi_6) & b_3 & \cos(\phi_5+\phi_6) & 1 \end{pmatrix}.$$

In the remaining cases 30–41, 43, 44 the absence of exceptional extreme matrices can be certified without computing the parametrization explicitly (see Sections 3.2, 3.3 below).

Along with the elements A_{ij} we also obtain expressions for the minimal zeros as functions of the angles ϕ_i. For reasons of limited space we shall not provide the expressions for the zeros, they can be deduced from their supports and Lemmas 3.1, 3.3.

In Section 3.3 below we shall further constrain the set of possible extremal matrices with a given minimal zero support set by using other conditions imposed by the copositivity of the matrix. However, first we shall consider special constellations of the index set $\mathcal{I}$, which immediately exclude the possibility of exceptional extremal matrices with this minimal zero support set.

3.2 Linear dependence of minimal zeros

In the previous section we parameterized the entries of the minimal zeros $u \in \mathcal{V}^A_{\min}$ corresponding to supports of cardinality 3 by angles ϕ_i. In some cases this allows to exclude the extremality of A immediately by virtue of the following result [17, Theorem 4.5].

Lemma 3.4. *A matrix $A \in \mathcal{COP}^n$ is not reduced with respect to the cone $\mathcal{S}^n_+$ if and only if* $\operatorname{span} \mathcal{V}^A_{\min} = \mathbb{R}^n$.

We now show that under some circumstances we may deduce the linear dependence of minimal zeros just from their supports. Suppose the minimal support set $\mathcal{V}^A_{\min}$ of a matrix $A \in \mathcal{COP}^n$ with unit diagonal

has a subset of the form

$$\{\{a,b,c\},\{a,b,d\},\{a,c,e\},\{a,d,e\}\},$$

where $I=\{a,\dots,e\}$ consists of 5 mutually distinct indices. Then by Lemma 3.3 the corresponding 5×5 sub-matrix A_I of A has the form

$$\begin{pmatrix} 1 & -\cos\phi_1 & -\cos\phi_2 & -\cos\phi_3 & -\cos\phi_4 \\ -\cos\phi_1 & 1 & \cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_3) & \star \\ -\cos\phi_2 & \cos(\phi_1+\phi_2) & 1 & \star & \cos(\phi_2+\phi_4) \\ -\cos\phi_3 & \cos(\phi_1+\phi_3) & \star & 1 & \cos(\phi_3+\phi_4) \\ -\cos\phi_4 & \star & \cos(\phi_2+\phi_4) & \cos(\phi_3+\phi_4) & 1 \end{pmatrix},$$

and the corresponding sub-vectors u_I of the minimal zeros u^1,u^2,u^3,u^4 are given by

$$\begin{pmatrix}\sin(\phi_1+\phi_2)\\ \sin\phi_2\\ \sin\phi_1\\ 0\\ 0\end{pmatrix},\ \begin{pmatrix}\sin(\phi_1+\phi_3)\\ \sin\phi_3\\ 0\\ \sin\phi_1\\ 0\end{pmatrix},\ \begin{pmatrix}\sin(\phi_2+\phi_4)\\ 0\\ \sin\phi_4\\ 0\\ \sin\phi_2\end{pmatrix},\ \begin{pmatrix}\sin(\phi_3+\phi_4)\\ 0\\ 0\\ \sin\phi_4\\ \sin\phi_3\end{pmatrix}$$

for some angles $\phi_1,\dots,\phi_4\in(0,\pi)$. The other components of the zeros all vanish.

It is now directly verified that these 4 zeros are linearly dependent, namely we have

$$\sin\phi_3\sin\phi_4 u^1-\sin\phi_2\sin\phi_4 u^2-\sin\phi_3\sin\phi_1 u^3+\sin\phi_2\sin\phi_1 u^4=0.$$

All coefficients are non-zero, hence every one of the 4 zeros can be represented as a linear combination of the other 3.

In this way we may establish linear dependencies of the minimal zeros of a copositive matrix just by examining its minimal zero support set. By removing a minimal zero which is linearly dependent on other zeros we do not change the span of the zeros. If after successive removing of zeros which are dependent on zeros which are still present we obtain a total number of zeros strictly smaller than the order of the matrix, then all minimal zeros must be contained in a proper subspace. By Lemma 3.4 the matrix is then not reduced with respect to the cone of positive semi-definite matrices and cannot be exceptional extremal.

In this way the absence of exceptional extremal matrices with minimal zero support set $\mathcal{I}$ can be certified in the cases 30–40 of Table 1.

In the case 42 a linear dependence between the six minimal zeros can be established by verifying that the determinant of the 6×6 matrix

$$\begin{pmatrix} \sin(\phi_1+\phi_2) & \sin\phi_3 & \sin\phi_4 & 0 & 0 & 0 \\ \sin\phi_2 & 0 & \sin(\phi_1+\phi_4) & 0 & \sin\phi_6 & 0 \\ 0 & 0 & \sin\phi_1 & \sin\phi_3 & \sin(\phi_4+\phi_6) & \sin(\phi_5+\phi_6) \\ 0 & \sin\phi_2 & 0 & \sin(\phi_3+\phi_5) & 0 & \sin\phi_6 \\ \sin\phi_1 & \sin(\phi_2+\phi_3) & 0 & \sin\phi_5 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sin\phi_4 & \sin\phi_5 \end{pmatrix}$$

formed column-wise of these zeros vanishes identically. In this case exceptional extremal matrices are also absent.

3.3 First order conditions

In Section 3.1 we parameterized the set of possible exceptional extremal matrices A with $\operatorname{supp}\mathcal{V}^A_{\min}=\mathcal{I}$ and their minimal zeros by a number of angles ϕ_i and a number of additional variables b_i, the latter corresponding to some entries of A which are uncovered by $\mathcal{I}$. In this section we obtain necessary conditions on these variables.

The analysis proceeds using equality and inequality relations generated by the minimal zeros corresponding to the given supports. If u is a zero of A, then the matrix-vector product Au has nonnegative entries [1, p.200]. Moreover, since $u^TAu=0$ is a scalar product of two nonnegative vectors, the i-th entry

of Au is zero whenever $u_i > 0$. The first order conditions $(Au)_j \geq 0,\ j = 1, \ldots, 6$, translate into non-strict inequalities on the parameters ϕ_i, b_i. While the angles ϕ_i enter the inequalities non-linearly, the resulting constraints on the b_i are linear with positive coefficients. The next result shows that the extremality condition together with the inequalities determine the elements b_i up to a finite number of possibilities.

Lemma 3.5. *Let $\mathcal{I} \subset 2^{\{1,\ldots,n\}}$ be an index set and let $A \in \mathcal{COP}^n$ be an exceptional extremal copositive matrix such that $A_{ii} = 1$ for all i and such that $\operatorname{supp} \mathcal{V}^A_{\min} = \mathcal{I}$. Let $\mathcal{B}$ be the set of all matrices $B \in \mathcal{S}^n$ such that $B_{ij} = A_{ij}$ for all elements A_{ij} covered by $\mathcal{I}$, and $Bu \geq 0$ for all minimal zeros $u \in \mathcal{V}^A_{\min}$.*

Then A is an extremal element of the polyhedron $\mathcal{B}$. In particular, there exists a subset of equalities $(Au^j)_k = 0$ which determine the values of the uncovered elements of A uniquely.

Proof. Assume that there exists $\Delta \in \mathcal{S}^n$ such that $A \pm \Delta \in \mathcal{B}$. If for some minimal zero u of A we have $(Au)_k = 0$, then by definition of $\mathcal{B}$ we get $(Au)_k \pm (\Delta u)_k = \pm(\Delta u)_k \geq 0$ and hence $(\Delta u)_k = 0$. Then by [12, Theorem 17] the matrix Δ is in the linear span of the face of A in $\mathcal{COP}^n$. But A is extremal, and therefore the face of A equals the ray generated by A. Hence Δ is proportional to A. Now the diagonal elements of any matrix $B \in \mathcal{B}$ equal 1. Since the diagonal elements are covered by $\mathcal{I}$, we have $\operatorname{diag} \Delta = \mathbf{0}$, and therefore $\Delta = 0$. Thus A is extremal in $\mathcal{B}$. This completes the proof. □

Since the polyhedron $\mathcal{B}$ has a finite number of extremal points, there exists a finite number of possible values of the variables b_i for fixed values of the variables ϕ_i. As a consequence, we obtain a finite number of (sub-)cases, in each of which the variables b_i are expressed explicitly as a function of the angles ϕ_i. In many cases the b_i are trigonometric functions of the angles, but in some cases they are more complicated ratios of trigonometric functions. In particular, such rational expressions appear in the extremal matrices corresponding to the minimal zero support sets 11 and 12 in Table 1.

In Table 3 we present the equalities $(Au^j)_k = 0$ determining the variables b_i for each of the cases 1–18, if there are any. The equalities given for case 19 are necessary to enforce extremality.

The inequalities $(Au^j)_k \geq 0$ not involving any of the elements b_i may lead to additional constraints on the variables ϕ_i. In many cases these constraints can be reduced to linear inequalities on the angles ϕ_i. In some other cases these constraints can be shown to hold automatically.

It may, however, also happen that these constraints are incompatible. We first state the following auxiliary result. Suppose the minimal support set $\mathcal{V}^A_{\min}$ of an extremal matrix $A \in \mathcal{COP}^n$ with unit diagonal has a subset of the form $\{\{a, b, c\}, \{b, c, d\}\}$, where $I = \{a, \ldots, d\}$ consists of 4 mutually distinct indices. Then by Lemma 3.3 the corresponding 4×4 sub-matrix A_I of A has the form

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & -\cos\phi_4 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 \\ -\cos\phi_4 & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 \end{pmatrix},$$

and the corresponding sub-vectors u_I of the minimal zeros u^1, u^2 are given by

$$\begin{pmatrix} \sin\phi_2 \\ \sin(\phi_1+\phi_2) \\ \sin\phi_1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ \sin\phi_3 \\ \sin(\phi_2+\phi_3) \\ \sin\phi_2 \end{pmatrix}$$

for some angles $\phi_1, \phi_2, \phi_3, \phi_4 \in (0, \pi)$ with $\phi_1 + \phi_2 < \pi$, $\phi_2 + \phi_3 < \pi$. The other components of the zeros all vanish. Then the condition $(A_I u_I^2)_a = \sin\phi_2(\cos(\phi_1+\phi_2+\phi_3) - \cos\phi_4) \geq 0$ yields $|\phi_1+\phi_2+\phi_3-\pi| \geq \pi-\phi_4$ and hence leads to the alternatives $\phi_1+\phi_2+\phi_3+\phi_4 \geq 2\pi$ or $\phi_1+\phi_2+\phi_3 \leq \phi_4$. We are now in a position to prove the following result.

Lemma 3.6. *Suppose the minimal support set $\mathcal{V}^A_{\min}$ of a matrix $A \in \mathcal{COP}^n$ with unit diagonal has a subset of the form $\{\{a, b, c\}, \{c, d, e\}, \{a, b, e\}, \{a, d, e\}\}$, where $I = \{a, \ldots, e\}$ consists of 5 mutually distinct*

indices. Then the corresponding submatrix A_I is of the form

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_5 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \star & \cos(\phi_1+\phi_5) \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) \\ \cos(\phi_4+\phi_5) & \star & -\cos\phi_3 & 1 & -\cos\phi_4 \\ -\cos\phi_5 & \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 \end{pmatrix}$$

with $\phi_1,\dots,\phi_5 > 0$ and $\sum_{i=1}^5 \phi_i \le \pi$.

Proof. The form of the matrix with $\phi_i \in (0,\pi)$ follows from Lemma 3.3. It remains to show the inequality $\sum_{i=1}^5 \phi_i \le \pi$.

Applying the above reasoning to the pair $\{\{e,a,b\},\{a,b,c\}\}$ of supports, we get the alternative $\phi_1 + \phi_2 + \phi_5 + \pi - \phi_3 - \phi_4 \ge 2\pi$ or $\phi_1 + \phi_2 + \phi_5 \le \pi - \phi_3 - \phi_4$. Applying it to the pair $\{\{c,d,e\},\{d,e,a\}\}$, we get $\phi_3 + \phi_4 + \phi_5 + \phi - \phi_1 - \phi_2 \ge 2\pi$ or $\phi_3 + \phi_4 + \phi_5 \le \phi - \phi_1 - \phi_2$. The first conditions of each pair are incompatible by virtue of $\phi_5 < \pi$, hence in at least one pair the second condition holds. This proves our claim. □

Applying Lemma 3.6 to appropriate subsets of the minimal zero support set 43 or 44 of Table 1 we establish that the constraints imposed by the lemma are incompatible, refuting the existence of copositive matrices with the corresponding minimal zero support set. Note that this still holds if the six supports are merely a subset of the full minimal zero support set, and the result is not limited to order 6.

In this section we established that the manifold of candidate exceptional extremal matrices A with unit diagonal and $\operatorname{supp} \mathcal{V}^A_{\min} = \mathcal{I}$ can be represented as a finite union of subsets, each of which is parameterized by a number of angles ϕ_i which are subject to linear and possibly non-linear constraints. In Section 3.5 below we obtain further constraints on the angles ϕ_i. However, first we shall show in the next section how to reduce the number of subsets.

3.4 Symmetry

In some cases the index set $\mathcal{I}$ remains invariant under a non-trivial subgroup of permutations of the indices $1,\dots,6$. This group will also act on the subsets of candidate exceptional extremal matrices corresponding to different extreme points of the polyhedron $\mathcal{B}$ from Lemma 3.5, permuting them. We then need to consider only one subset per orbit of the group action. We may implement this by imposing additional non-strict inequalities on the parameters ϕ_i which can be enforced by applying an appropriate group element.

In the cases 1, 11, 14, 15, 17, 18 of Table 1 there is only one subset which is itself invariant under the action of the non-trivial symmetry group.

In the cases 2, 3, 5–8, 16, 19 we can reduce the initially larger number of subsets to one.

In case 9 the symmetry group is trivial, while the number of subsets is two. This case hence decomposes into two non-isomorphic sub-cases.

In case 13 the symmetry group is non-trivial, but reduces the number of subsets only to two, and here we also get two non-isomorphic sub-cases. The manifolds corresponding to these sub-cases intersect in a submanifold of lower dimension.

In Table 4 we list the generators and types of the non-trivial symmetry groups of those minimal zero support sets which are realized by exceptional extremal copositive matrices and provide the additional inequalities on the angle parameters ϕ_i.

3.5 Copositivity and absence of additional minimal zeros

In this section we check which of the remaining candidate matrices are indeed copositive. In order to check copositivity we use a criterion described in [8]. We show that this method can also be adapted to check, for a given copositive matrix, the presence or absence of minimal zeros with a given support set. In this way we ensure that the extremal matrices found for a given minimal zero support set $\mathcal{I}$ indeed do not possess minimal zeros with additional support sets.

3.5.1 Copositivity

The aforementioned copositivity criterion is based on the following result.

Theorem 3.7. *[8, Theorem 4.6] For $A \in \mathcal{S}^n$ we have that $A \in \mathcal{COP}^n$ if and only if for every non-empty index set $I \subset \{1, \dots, n\}$, there exists $v \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ with $\operatorname{supp} v \subseteq I \subseteq \operatorname{supp}_{\geq 0}(Av)$.*

Corollary 3.8. *A matrix $A \in \mathcal{S}^n$ is copositive if and only if for every non-empty index set $I \subset \{1, \dots, n\}$, the submatrix A_I is copositive or there exists $v \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ with $\operatorname{supp} v \subseteq I \subseteq \operatorname{supp}_{\geq 0}(Av)$.*

Proof. The forward implication follows directly from the forward implication in Theorem 3.7.

Let us show the reverse implication. Suppose that A_I is copositive for some index set I. By Theorem 3.7 there exists $\tilde{v} \in \mathbb{R}^{|I|} \setminus (-\mathbb{R}^{|I|}_+)$ with $\operatorname{supp} \tilde{v} \subseteq \{1, \dots, |I|\} \subseteq \operatorname{supp}_{\geq 0}(A_I \tilde{v})$. Padding $\tilde{v}$ with $n - |I|$ zeros at appropriate places, we obtain $v \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ with $\operatorname{supp} v \subseteq I \subseteq \operatorname{supp}_{\geq 0}(Av)$. Now the proof is completed by applying the reverse implication in Theorem 3.7. □

This implies that for each non-empty index set $I \in \{1, \dots, 6\}$ we have either to find a vector $v \in \mathbb{R}^6$ such that I contains the support of v and is contained in the nonnegative support of Av, or to prove that the submatrix A_I is copositive.

For I of size 1 or 2 we may take $v = \sum_{i \in I} e_i$, because the diagonal elements of A equal 1 and are greater or equal than the non-diagonal elements.

For I containing the support of a minimal zero u we may take $v = u$, as in this case we have $I \subset \{1, \dots, 6\} = \operatorname{supp}_{\geq 0} u$. The equality is ensured by the conditions $(Au)_j \geq 0$ considered in Section 3.3.

For index sets I of cardinality 3 we check copositivity of A_I by the following criterion, which amounts to a linear inequality constraint on the angles ϕ_i.

Lemma 3.9. *Let*

$$A = \begin{pmatrix} 1 & -\cos\phi_1 & -\cos\phi_2 \\ -\cos\phi_1 & 1 & -\cos\phi_3 \\ -\cos\phi_2 & -\cos\phi_3 & 1 \end{pmatrix} \in \mathcal{S}^3$$

with $\phi_1, \phi_2, \phi_3 \in [0, \pi]$. Then A is copositive if and only if $\phi_1 + \phi_2 + \phi_3 \geq \pi$.

Proof. The claim follows from the strict monotonicity of the function $\phi \mapsto -\cos\phi$ on $[0, \pi]$ and [10, Lemma 4.7]. □

For index sets of size 4 we provide a vector v for each case individually or prove that it does not exist. These vectors are listed in Table 5.

Index sets of cardinality 5 or 6 turn always out to be supersets of a minimal zero support.

It turns out that the additional constraints on the angles ϕ_i imposed by the copositivity of A further reduce the set of ϕ_i in a way such that the non-linear constraints on the ϕ_i found in Section 3.3 become redundant. As a consequence, the set of possible values of the angles ϕ_i is again reduced to a polytope.

3.5.2 Absence of additional minimal zeros

We also have to certify the absence of minimal zeros with additional support sets. We shall use the following result, which is also of independent interest.

Lemma 3.10. *Let $A \in \mathcal{COP}^n$ and let w be a minimal zero of A with support set I. Let $u \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ be such that $\operatorname{supp} u \subset I \subset \operatorname{supp}_{\geq 0}(Au)$. Set $B = A_I$ and $v = u_I$. Then v is proportional to w_I with a positive proportionality constant and $Bv = 0$.*

Proof. The condition $\operatorname{supp} u \subset I$ implies that v has at least one positive element. Further $Bv = (Au)_I \geq 0$ by virtue of $I \subset \operatorname{supp}_{\geq 0}(Au)$.

Since w is a minimal zero of A, the submatrix B is positive semi-definite of co-rank 1 and with positive kernel vector w [17, Lemma 3.7]. Hence $Bw = 0$ and we obtain $v^T B w = 0$. But $Bv \geq 0$ and $w > 0$, which implies also $Bv = 0$ and proves our second claim. It follows also that the vector v is in the kernel of B and must hence be proportional to the kernel vector w. The proportionality constant is positive because v has a positive element. This completes the proof. □

Suppose we intend to check the absence of a minimal zero with support set I. In the previous section we obtained a vector $u \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ such that $\operatorname{supp} u \subset I \subset \operatorname{supp}_{\geq 0}(Au)$. Set $B = A_I$ and $v = u_I$. If v has not all elements positive or if $Bv \neq 0$, then this certifies the absence of a minimal zero with support I.

In this way the absence of additional minimal zeros with support sets I of cardinality 4 or more is certified for all occurring cases. For support sets $I = \{i, j, k\}$ of cardinality 3 the absence of minimal zeros can in many cases be certified by virtue of Lemma 3.3 by verifying the strict inequality $\phi_i + \phi_j + \phi_k > \pi$, where the angles are defined in the formulation the lemma. In other cases this inequality has to be added as a constraint. In the remaining cases only the equality $\phi_i + \phi_j + \phi_k = \pi$ is possible, which leads to the conclusion that a minimal zero with support I does indeed exist. In particular, this excludes the possibility of extremal copositive matrices having the minimal zero support sets 21–29 in Table 1. In case 20 this possibility is excluded by the appearance of additional minimal zeros with support of cardinality two. The appearing additional support sets are listed in Table 6.

Having verified the copositivity and the absence of additional minimal zeros, it remains to check extremality of the remaining candidate matrices.

3.6 Extremality

In the previous sections we obtained a manifold of copositive matrices with a given minimal zero support set $\mathcal{I}$, parameterized by a number of angles ϕ_i varying in a polytope. The last step towards the classification of the extreme rays is to check extremality of these matrices. First we provide an extremality criterion for copositive matrices [12, Theorem 17].

Theorem 3.11. *Let $A \in \mathcal{COP}^n$. Then A is not extremal if and only if there exists a matrix $B \in \mathcal{S}^n$, not proportional to A, such that $(Bu)_i = 0$ for all $u \in \mathcal{V}^A_{\min}$, $i \notin \operatorname{supp}(Au)$.*

In other words, given A we consider the linear system of equations $\{(Bu)_i = 0 \,|\, u \in \mathcal{V}^A_{\min},\ (Au)_i = 0\}$ on B. Clearly all multiples of A are solutions of this system. If there are further solutions, i.e., the dimension of the solution space is at least 2, then A is not extremal.

The coefficient matrix of the linear system consists of elements of the minimal zeros $u \in \mathcal{V}^A_{\min}$ and hence depends on the angles ϕ_i. For different values of the ϕ_i the system may be different, because some of the inequalities $(Au)_i \geq 0$ considered in Section 3.3 may become equalities at the boundary of the polytope of angles, in which case the corresponding equations $(Bu)_i = 0$ are added to the system. Each of these cases necessitates a separate consideration.

In some cases special considerations lead directly to the conclusion that the manifold of candidate matrices A consists of extreme rays. In particular, this is the case if there are 5 minimal zero supports of cardinality 3, with its union I being of cardinality 5, and which are arranged in a cyclic manner (cases 11, 15, 16, 18 in Table 1). In this case the corresponding 5×5 submatrix A_I is extremal in $\mathcal{COP}^5$ [16]. Hence B_I is proportional to A_I by the relations $(Bu)_i = 0$ involving the 5 minimal zeros. The remaining relations are then easily verified to determine the remaining entries of B uniquely.

However, in most cases the dimension of the system is too large to determine its rank directly. We therefore apply a technique to reduce the dimension of the system, which is a development of the method introduced in [18] and which may also be of independent interest.

We are given a system of linear equations $(Bu^j)_i = 0$ on a matrix $B \in \mathcal{S}^n$, where $u^j \in \mathbb{R}^n$, $j = 1, \ldots, m$ are some vectors and the index pairs (i, j) vary in some subset $\mathcal{J} \subset \{1, \ldots, n\} \times \{1, \ldots, m\}$. As such the system has $\frac{n(n+1)}{2}$ independent variables, namely the entries of B.

Let $F \in \mathbb{R}^{n \times r}$ be a matrix, and let $J \subset \{j \in \{1, \ldots, m\} \,|\, F^T u^j = 0\}$. Suppose further that there exists a subset $I \subset \{1, \ldots, n\}$ of cardinality r such that the corresponding submatrix F' of F is invertible. We now make a linear change of variables, replacing the $\frac{r(r+1)}{2}$ entries of the principal submatrix B_I by the entries of $P = (F')^{-1} B_I (F')^{-T} \in \mathcal{S}^r$. Then $B_I = (FPF^T)_I$ is a linear function of P.

We now use some of the equations to express more entries of B as a function of P, namely by representing them as the corresponding entries of the product $X = FPF^T$. We proceed step by step. Suppose at some stage there exists $(i, j) \in \mathcal{J}$, corresponding to an equation $(Bu^j)_i = 0$ of the system, and $k \in \operatorname{supp} u^j$ such that $j \in J$, and all variables B_{il}, $l \in \operatorname{supp} u^j \setminus \{k\}$, have already been expressed as the corresponding entries of X. Then the relation $(Xu^j)_i = 0$, which holds by definition of J, implies that also $B_{ik} = X_{ik}$. We may

thus eliminate the equation $(Bu^j)_i = 0$ from the system and add the element B_{ik} to the list of entries of B which have been expressed by the corresponding entries of X as linear functions of P.

If not all equations can be used, we may restart the process with a new matrix product $Y = GQG^T$, choosing the factor G appropriately. We end up with a fewer number of independent variables, namely the entries of the central factors $P, Q, \ldots$. Some elements B_{ik} may have been expressed as both X_{ik} and Y_{ik}. In this case we have to add the corresponding relations $X_{ik} = Y_{ik}$ to the system of equations, which become equations on the entries of P and Q.

A concrete example to illustrate the method will be given in Section 4.5 further below.

In our situation it was in all cases sufficient to use at most two products $X = FPF^T$, $Y = GQG^T$, with the central factors P, Q being of size 2×2 and possibly a few of the original equations $(Bu^j)_i = 0$ and entries B_{ik} remaining as relations and independent variables, respectively. The factors F, G are chosen as appropriate functions of the angles ϕ_i in order to be orthogonal to as many minimal zeros u^j as possible. The dimension of the solution space can then be determined by further transformations of the now low-dimensional coefficient matrix.

In cases 1–5, 11, 12, 17, 18 the matrices corresponding to the interior of the polytope of possible angles ϕ_i are exactly those which are extremal. In cases 7, 8, 13, 15, 16 parts of the boundary of the polytope also correspond to extremal matrices, while in cases 7–10, 13 there exist submanifolds in the interior of the polytope corresponding to non-extremal matrices. The exact expressions for each case are presented in Section 5.

4 Special cases

In this section we consider the two minimal zero support sets in Table 1 which contain supports of cardinality 4.

Copositive matrices with minimal zero support set 41 of Table 1 fall into the framework considered in [18]. They are either positive semi-definite or a sum of a positive semi-definite rank 1 matrix and an exceptional extremal copositive matrix with minimal zero support set 13 of Table 1 [18, Theorem 5.12]. Hence case 41 does not yield exceptional extremal copositive matrices, and the minimal zeros of matrices with this minimal zero support set are necessarily linearly dependent.

Let us consider case 19 of Table 1.

4.1 Auxiliary results

In this section we provide some results on 4×4 positive semi-definite matrices with a positive kernel vector. This will be of use since the presence of the minimal zero support $\{2, 3, 4, 6\}$ implies that the corresponding principal submatrix of A is of this form.

Lemma 4.1. *Let $A \in \mathcal{S}^4_+$ be of rank 3 with positive kernel vector u, with unit diagonal, and with off-diagonal elements $A_{ij} = -\cos\phi_{ij}$, $\phi_{ij} \in (0, \pi)$. Suppose further that $\phi_{12} + \phi_{23} < \pi$. Then*

$$\sin\phi_{23}\cos\phi_{14} + \sin(\phi_{12} + \phi_{23})\cos\phi_{24} + \sin\phi_{12}\cos\phi_{34} > 0.$$

Proof. Define the vector $v = (\sin\phi_{23}, \sin(\phi_{12} + \phi_{23}), \sin\phi_{12}, 0)^T$. Let also $\delta = A_{13} - \cos(\phi_{12} + \phi_{23})$. Then $\delta > 0$, because $A_{\{1,2,3\}} \succ 0$. It also follows that $Av = (\delta\sin\phi_{12}, 0, \delta\sin\phi_{23}, \star)^T$.

We have $u^T Av = 0$ and hence

$$u_4(Av)_4 = -\delta(u_1\sin\phi_{12} + u_3\sin\phi_{23}) < 0.$$

It follows that $(Av)_4 < 0$, which yields the desired claim. □

Lemma 4.2. *Let $B \in \mathcal{S}^4$ be a partially defined matrix with three undetermined elements B_{13}, B_{14}, B_{24} and let $u \in \mathbb{R}^4_{++}$ be a vector. Then there exists a completion of B such that $Bu = 0$ if and only if*

$$B_{11}u_1^2 + 2B_{12}u_1u_2 + B_{22}u_2^2 = B_{33}u_3^2 + 2B_{34}u_3u_4 + B_{44}u_4^2.$$

In this case the completion is unique.

Proof. The condition $Bu = 0$ is equivalent to the linear system

$$\begin{pmatrix} B_{11}u_1 + B_{12}u_2 & u_3 & u_4 & \\ B_{12}u_1 + B_{22}u_2 + B_{23}u_3 & & & u_4 \\ B_{23}u_2 + B_{33}u_3 + B_{34}u_4 & u_1 & & \\ B_{34}u_3 + B_{44}u_4 & & u_1 & u_2 \end{pmatrix} \begin{pmatrix} 1 \\ B_{13} \\ B_{14} \\ B_{24} \end{pmatrix} = 0$$

on the unknown matrix elements. Thus there exists a completion if and only if the determinant of the coefficient matrix vanishes. After removing non-vanishing factors we arrive at the condition in the formulation of the lemma.

The positivity of the elements u_i guarantees that the matrix elements are determined uniquely. □

Lemma 4.3. *Let $B \in \mathcal{S}^4$ be a partially defined matrix with two undetermined elements B_{13}, B_{24} and let $u \in \mathbb{R}^4_{++}$ be a vector. Then there exists a completion of B such that $Bu = 0$ if and only if in addition to the condition in Lemma 4.2 the condition*

$$B_{11}u_1^2 + 2B_{14}u_1u_4 + B_{44}u_4^2 = B_{22}u_2^2 + 2B_{23}u_2u_3 + B_{33}u_3^2$$

holds. In this case the completion is unique.

Proof. The condition $Bu = 0$ is equivalent to the linear system

$$\begin{pmatrix} B_{11}u_1 + B_{12}u_2 + B_{14}u_4 & u_3 & \\ B_{12}u_1 + B_{22}u_2 + B_{23}u_3 & & u_4 \\ B_{23}u_2 + B_{33}u_3 + B_{34}u_4 & u_1 & \\ B_{14}u_1 + B_{34}u_3 + B_{44}u_4 & & u_2 \end{pmatrix} \begin{pmatrix} 1 \\ B_{13} \\ B_{24} \end{pmatrix} = 0$$

on the unknown matrix elements. The coefficient matrix has deficient rank if and only if the two conditions in the Lemmas hold.

The positivity of the elements u_i again guarantees that the matrix elements are determined uniquely. □

We have also the following result, which is a special case of [17, Lemma 5.6 (d)].

Lemma 4.4. *Let $A \in \mathcal{COP}^4$ have unit diagonal and suppose there exists a minimal zero of A with support of cardinality 4. Let the off-diagonal elements of A be given by $A_{ij} = -\cos\phi_{ij}$, $\phi_{ij} \in [0, \pi]$. Then for every three pair-wise distinct indices $i, j, k \in \{1, 2, 3, 4\}$ we have $\phi_{ij} + \phi_{ik} + \phi_{jk} > \pi$ and $\phi_{ij} + \phi_{ik} - \phi_{jk} < \pi$.*

We may now proceed to the study of copositive matrices with minimal zero support set 19 of Table 1.

4.2 Parametrization

As outlined in Section 3.1 we may use the minimal zero supports of cardinality 3 to express entries of a copositive matrix A with unit diagonal and the considered minimal zero support set by some angles ϕ_i. From the five supports $\{3, 4, 5\}, \{1, 4, 5\}, \{1, 2, 5\}, \{1, 2, 3\}, \{1, 5, 6\}$ we get

$$A = \begin{pmatrix} 1 & -\cos\phi_4 & \cos(\phi_4 + \phi_5) & \cos(\phi_2 + \phi_3) & -\cos\phi_3 & \cos(\phi_3 + \phi_6) \\ -\cos\phi_4 & 1 & -\cos\phi_5 & A_{24} & \cos(\phi_3 + \phi_4) & -\cos\phi_7 \\ \cos(\phi_4 + \phi_5) & -\cos\phi_5 & 1 & -\cos\phi_1 & \cos(\phi_1 + \phi_2) & -\cos\phi_8 \\ \cos(\phi_2 + \phi_3) & A_{24} & -\cos\phi_1 & 1 & -\cos\phi_2 & -\cos\phi_9 \\ -\cos\phi_3 & \cos(\phi_3 + \phi_4) & \cos(\phi_1 + \phi_2) & -\cos\phi_2 & 1 & -\cos\phi_6 \\ \cos(\phi_3 + \phi_6) & -\cos\phi_7 & -\cos\phi_8 & -\cos\phi_9 & -\cos\phi_6 & 1 \end{pmatrix} \tag{1}$$

with the angles $\phi_i \in (0, \pi)$ satisfying the conditions $\sum_{i=1}^5 \phi_i \leq \pi$ (by Lemma 3.6), $\phi_3 + \phi_6 < \pi$.

The minimal zeros $u^1, \ldots, u^6$ can be represented as the columns of the matrix

$$\begin{pmatrix} 0 & \sin\phi_2 & \sin(\phi_3 + \phi_4) & \sin\phi_5 & \sin\phi_6 & 0 \\ 0 & 0 & \sin\phi_3 & \sin(\phi_4 + \phi_5) & 0 & u_{62} \\ \sin\phi_2 & 0 & 0 & \sin\phi_4 & 0 & u_{63} \\ \sin(\phi_1 + \phi_2) & \sin\phi_3 & 0 & 0 & 0 & u_{64} \\ \sin\phi_1 & \sin(\phi_2 + \phi_3) & \sin\phi_4 & 0 & \sin(\phi_3 + \phi_6) & 0 \\ 0 & 0 & 0 & 0 & \sin\phi_3 & u_{66} \end{pmatrix}, \tag{2}$$

where $u_{62}, u_{63}, u_{64}, u_{66} > 0$.

4.3 First order conditions

In this section we investigate the conditions $(Au^i)_j \geq 0$ for $j \notin \operatorname{supp}\{u^i\}$. It will turn out that most of these inequalities have to be strict.

The presence of the minimal zero support $\{2,3,4,6\}$ implies that all proper principal submatrices of $A_{\{2,3,4,6\}}$ are positive definite [17, Corollary 3.8].

The conditions $(Au^5)_2 \geq 0$, $(Au^5)_4 \geq 0$ yield $-\cos(\phi_2-\phi_6)-\cos\phi_9 \geq 0$, $\cos(\phi_3+\phi_4+\phi_6)-\cos\phi_7 \geq 0$ and hence either $\pi+\phi_6 \leq \phi_2+\phi_9$ or $\phi_6+\phi_9 \geq \pi+\phi_2$, and either $\phi_3+\phi_4+\phi_6 \leq \phi_7$ or $\phi_3+\phi_4+\phi_6+\phi_7 \geq 2\pi$.

From the copositivity of $A_{\{3,5,6\}}$ we get $\phi_6+\phi_8+\pi-\phi_1-\phi_2 > \pi$, while by virtue of Lemma 4.4 applied to the submatrix $A_{\{3,4,6\}}$ we obtain $\phi_8+\phi_9-\phi_1 < \pi$. These inequalities combined exclude the possibility $\pi+\phi_6 \leq \phi_2+\phi_9$.

Likewise, copositivity of $A_{\{1,3,6\}}$ yields $\phi_8+\pi-\phi_4-\phi_5+\pi-\phi_3-\phi_6 > \pi$, while Lemma 4.4 applied to the submatrix $A_{\{2,3,6\}}$ implies $-\phi_5+\phi_7+\phi_8 < \pi$. These inequalities combined exclude the possibility $\phi_3+\phi_4+\phi_6+\phi_7 \geq 2\pi$.

Hence $\phi_6+\phi_9 \geq \pi+\phi_2$ and $\phi_3+\phi_4+\phi_6 \leq \phi_7$. We shall now show that these conditions imply $(Au^i)_j > 0$ for all other pairs (i,j) with $j \neq \operatorname{supp} u^i$.

Lemma 4.5. *Let A be given by (1) and let $u^1,\dots,u^6$ be given by the columns of (2) with $\phi_i \in (0,\pi)$, $\phi_1+\dots+\phi_5 \leq \pi$, $A_{\{2,3,4\}} \succ 0$, $u_{62},u_{63},u_{64},u_{66} > 0$, $A_{\{2,3,4,6\}}u^6_{\{2,3,4,6\}} = 0$, $\phi_6+\phi_9 \geq \pi+\phi_2$, $\phi_3+\phi_4+\phi_6 \leq \phi_7$.*

Then $(Au^5)_{\{2,4\}}, (Au^2)_6, (Au^3)_6 \geq 0$, $(Au^1)_{\{1,2,6\}}, (Au^2)_{\{2,3\}}, (Au^3)_{\{3,4\}}, (Au^4)_{\{4,5,6\}}, (Au^5)_3, (Au^6)_{\{1,5\}} > 0$, and $\phi_1+\dots+\phi_5 < \pi$.

Proof. Note that the symmetry $(123456) \mapsto (543216)$, which also acts on the zeros by $u^1 \leftrightarrow u^4$, $u^2 \leftrightarrow u^3$ and on the angles by $\phi_2 \leftrightarrow \phi_4$, $\phi_1 \leftrightarrow \phi_5$, $\phi_7 \leftrightarrow \phi_9$, $\phi_6 \mapsto \pi-\phi_3-\phi_6$, leaves the conditions and the assertions in the lemma invariant.

The submatrix $A_{\{2,3,4,6\}}$ is PSD of rank 3 with a positive kernel vector. In particular, all its proper principal submatrices are positive definite. Note also that Lemma 4.4 is applicable to $A_{\{2,3,4,6\}}$.

From $\phi_6-\phi_2 \geq \pi-\phi_9$ we have $\cos(\phi_6-\phi_2)+\cos\phi_9 \leq 0$ and $(Au^5)_4, (Au^2)_6 \geq 0$. Likewise, $\phi_7 \geq \phi_3+\phi_4+\phi_6$ gives $\cos(\phi_3+\phi_4+\phi_6)-\cos\phi_7 \geq 0$ and hence $(Au^5)_2, (Au^3)_6 \geq 0$.

Define $\delta_{13} = A_{13}+\cos(\phi_1+\phi_2+\phi_3)$, $\delta_{36} = A_{36}+\cos(\phi_1+\phi_2-\phi_6)$, $\delta_{46} = A_{46}-\cos(\phi_6-\phi_2)$. Then we get

$$A_{\{1,3,4,5,6\}} = \begin{pmatrix} 1 & 0 \\ -\cos(\phi_1+\phi_2+\phi_3) & -\sin(\phi_1+\phi_2+\phi_3) \\ \cos(\phi_2+\phi_3) & \sin(\phi_2+\phi_3) \\ -\cos\phi_3 & -\sin\phi_3 \\ \cos(\phi_3+\phi_6) & \sin(\phi_3+\phi_6) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\cos(\phi_1+\phi_2+\phi_3) & -\sin(\phi_1+\phi_2+\phi_3) \\ \cos(\phi_2+\phi_3) & \sin(\phi_2+\phi_3) \\ -\cos\phi_3 & -\sin\phi_3 \\ \cos(\phi_3+\phi_6) & \sin(\phi_3+\phi_6) \end{pmatrix}^T + \begin{pmatrix} 0 & \delta_{13} & 0 & 0 & 0 \\ \delta_{13} & 0 & 0 & 0 & \delta_{36} \\ 0 & 0 & 0 & 0 & \delta_{46} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \delta_{36} & \delta_{46} & 0 & 0 \end{pmatrix}.$$

By virtue of $\phi_1+\dots+\phi_5 \leq \pi$ we have $\delta_{13} \geq 0$, by virtue of $\phi_6+\phi_9 \geq \pi+\phi_2$ we have $\delta_{46} \geq 0$.

The submatrix

$$A_{\{3,4,6\}} = \begin{pmatrix} -\cos(\phi_1+\phi_2) & -\sin(\phi_1+\phi_2) \\ \cos\phi_2 & \sin\phi_2 \\ \cos\phi_6 & \sin\phi_6 \end{pmatrix} \begin{pmatrix} -\cos(\phi_1+\phi_2) & -\sin(\phi_1+\phi_2) \\ \cos\phi_2 & \sin\phi_2 \\ \cos\phi_6 & \sin\phi_6 \end{pmatrix}^T + \begin{pmatrix} 0 & 0 & \delta_{36} \\ 0 & 0 & \delta_{46} \\ \delta_{36} & \delta_{46} & 0 \end{pmatrix}$$

is positive definite, which implies

$$\begin{pmatrix} \cos\phi_6 \\ \sin\phi_6 \end{pmatrix}^T \begin{pmatrix} -\cos(\phi_1+\phi_2) & -\sin(\phi_1+\phi_2) \\ \cos\phi_2 & \sin\phi_2 \end{pmatrix}^{-1} \begin{pmatrix} \delta_{36} \\ \delta_{46} \end{pmatrix} = \frac{\sin(\phi_2-\phi_6)\delta_{36}+\sin(\phi_1+\phi_2-\phi_6)\delta_{46}}{\sin\phi_1} < 0.$$

From $\phi_6 + \phi_9 \geq \pi + \phi_2$ we have $\phi_6 > \phi_2$ and $\sin(\phi_6 - \phi_2) > 0$. Hence

$$\delta_{36} > \frac{\sin(\phi_1 + \phi_2 - \phi_6)\delta_{46}}{\sin(\phi_6 - \phi_2)}. \tag{3}$$

We then have

$$(Au^5)_3 = \sin\phi_6\delta_{13} + \sin\phi_3\delta_{36} > \sin\phi_6\delta_{13} + \sin\phi_3\frac{\sin(\phi_1 + \phi_2 - \phi_6)\delta_{46}}{\sin(\phi_6 - \phi_2)}.$$

Therefore, if $\phi_1 + \phi_2 - \phi_6 \geq 0$, then $(Au^5)_3 > 0$.

Applying the symmetry, we get $(Au^5)_3 > 0$ also in the case $\phi_3 + \phi_4 + \phi_5 + \phi_6 \geq \pi$.

Let us now assume that $\phi_1 + \phi_2 < \phi_6$, $\phi_4 + \phi_5 < \pi - \phi_3 - \phi_6$. Then

$$\begin{aligned}(Au^5)_3 &= \cos(\phi_4 + \phi_5)\sin\phi_6 + \cos(\phi_1 + \phi_2)\sin(\phi_3 + \phi_6) + A_{36}\sin\phi_3 \\ &> \cos(\pi - \phi_3 - \phi_6)\sin\phi_6 + \cos\phi_6\sin(\phi_3 + \phi_6) - \sin\phi_3 = 0.\end{aligned}$$

Hence in any case $(Au^5)_3 > 0$.

Further we have by virtue of (3)

$$\begin{aligned}(Au^1)_6 &= \sin\phi_2\delta_{36} + \sin(\phi_1 + \phi_2)\delta_{46} > \frac{\sin\phi_2\sin(\phi_1 + \phi_2 - \phi_6) + \sin(\phi_1 + \phi_2)\sin(\phi_6 - \phi_2)}{\sin(\phi_6 - \phi_2)}\delta_{46} \\ &= \frac{\sin\phi_1\sin\phi_6}{\sin(\phi_6 - \phi_2)}\delta_{46} \geq 0.\end{aligned}$$

By symmetry we also get $(Au^4)_6 > 0$.

Further we have

$$(Au^4)_4 = (\cos(\phi_2 + \phi_3) + \cos(\phi_1 + \phi_4 + \phi_5))\sin\phi_5 + \sin(\phi_4 + \phi_5)(A_{24} - \cos(\phi_1 + \phi_5)) > 0,$$

$$(Au^2)_2 = \sin\phi_3(A_{24} - \cos(\phi_1 + \phi_5) + \cos(\phi_2 + \phi_3 + \phi_4) + \cos(\phi_1 + \phi_5)) > 0,$$

because $A_{24} > \cos(\phi_1 + \phi_5)$. Likewise $(Au^1)_2, (Au^3)_4 > 0$ by symmetry.

Define $\delta_{14} = A_{14} - \frac{-\sin(\phi_4+\phi_5)A_{24} + \sin\phi_4\cos\phi_1}{\sin\phi_5}$, $\delta_{16} = A_{16} - \frac{\sin(\phi_4+\phi_5)\cos\phi_7 + \sin\phi_4\cos\phi_8}{\sin\phi_5}$. Then

$$A_{\{1,2,3,4,6\}} = P + \delta_{14}E_{14} + \delta_{16}E_{15}, \tag{4}$$

where $P \in \mathcal{S}^5$ is such its submatrices $P_{\{2,3,4,5\}}, P_{\{1,2,3\}}$ are PSD of co-rank 1 and $Pu^4_{\{1,2,3,4,6\}} = 0$. Hence P is PSD of rank 3 and $Pu^6_{\{1,2,3,4,6\}} = 0$. We then get

$$0 < (Au^4)_4 = \delta_{14}\sin\phi_5, \qquad 0 < (Au^4)_6 = \delta_{16}\sin\phi_5,$$

and hence $\delta_{14}, \delta_{16} > 0$. It follows that

$$(Au^6)_1 = \delta_{14}u_{64} + \delta_{16}u_{66} > 0.$$

By symmetry we also get $(Au^6)_5 > 0$.

Now by Lemma 4.1, applied to the submatrix $A_{\{2,3,4,6\}}$, we have

$$\cos\phi_7\sin\phi_1 + \cos\phi_8\sin(\phi_1 + \phi_5) + \cos\phi_9\sin\phi_5 > 0.$$

By virtue of Lemma 4.4 applied to $A_{\{2,3,6\}}$ we have $|\pi - \phi_5 - \phi_7| < \phi_8$ and hence $\cos\phi_8 < -\cos(\phi_5 + \phi_7)$. Substituting into the above inequality we obtain

$$\cos\phi_7\sin\phi_1 - \cos(\phi_5 + \phi_7)\sin(\phi_1 + \phi_5) + \cos\phi_9\sin\phi_5 = (\cos\phi_9 - \cos(\phi_1 + \phi_5 + \phi_7))\sin\phi_5 > 0.$$

This yields $|\phi_1 + \phi_5 + \phi_7 - \pi| < \pi - \phi_9$ and therefore

$$\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 + \pi = \phi_1 + \phi_5 + (\phi_3 + \phi_4 + \phi_6) + (\pi + \phi_2 - \phi_6) \leq \phi_1 + \phi_5 + \phi_7 + \phi_9 < 2\pi.$$

This finally gives $\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 < \pi$ and hence also $(Au_1)_1, (Au_2)_3, (Au_3)_3, (Au_4)_5 > 0$.

This completes the proof. □

4.4 Copositivity

Let us now show that the same conditions already guarantee the copositivity of A.

Lemma 4.6. *Let the matrix A be as in Lemma 4.5. Then A is copositive, exceptional, and there are no other minimal zeros than the multiples of $u^1, \dots, u^6$.*

Proof. From Lemma 4.5 we have that $\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 < \pi$ and $Au^i \geq 0$ for $i = 1, \dots, 6$.

By definition $A_{\{1,2,3,4,5\}}$ is the sum of an extremal copositive matrix [16] and a positive multiple of E_{24}. In particular, this submatrix is copositive.

By (4) we have that the submatrix $A_{\{1,2,3,4,6\}}$ is in $\mathcal{S}^5_+ + \mathcal{N}^5$. By symmetry this holds also for $A_{\{2,3,4,5,6\}}$.

Let us prove the copositivity of A. Every subset $I \subset \{1, \dots, 6\}$ is either a subset of $\{1, 2, 3, 4, 5\}$ or $\{1, 2, 3, 4, 6\}$ or $\{2, 3, 4, 5, 6\}$ or a super set of $\{1, 5, 6\}$. Thus the copositivity of A follows from Corollary 3.8, where for $I \supset \{1, 5, 6\}$ we choose $v = u^5$.

The submatrices $A_{\{1,2,3,4,5\}}, A_{\{1,2,3,4,6\}}, A_{\{2,3,4,5,6\}}$ do not have zeros other than multiples of u^i by construction. For strict supersets $I \supset \{1, 5, 6\}$ there cannot be a minimal zero with support I because $\operatorname{supp} u^5$ is a strict subset of I. Hence there are no additional minimal zeros.

Let us show that A is exceptional. We have that A is reduced with respect to $\mathcal{N}^6$ by [17, Lemma 4.1], because the minimal zero support set covers all elements of A. Hence if A is not exceptional, it must be PSD. But then $Au^i = 0$ for all $i = 1, \dots, 6$, which is in contradiction to Lemma 4.5.

This completes the proof. □

We have proven the following result.

Lemma 4.7. *Let the matrix $A \in \mathcal{COP}^6$ have unit diagonal elements and let its minimal zero support set be given by the index set 19 in Table 1. Then there exist $\phi_1, \dots, \phi_6 \in (0, \pi)$ and $u_{62}, u_{63}, u_{64}, u_{66} > 0$, satisfying $\phi_1 + \dots + \phi_5 < \pi$, $\phi_3 + \phi_4 + \phi_6 < \pi$, $\phi_6 > \phi_2$, such that the minimal zeros $u^1, \dots, u^6$ of A are given by the columns of the matrix* (2).

Moreover, given $u^1, \dots, u^6$ as above, a matrix $A \in \mathcal{S}^6$ with unit diagonal elements is copositive exceptional with minimal zeros $u^1, \dots, u^6$ if and only if it is of the form (1) *and satisfies $A_{\{2,3,4\}} \succ 0$, $A_{\{2,3,4,6\}} u^6_{\{2,3,4,6\}} = 0$, $\phi_7, \phi_8, \phi_9 \in (0, \pi)$, $\phi_6 + \phi_9 \geq \pi + \phi_2$, $\phi_3 + \phi_4 + \phi_6 \leq \phi_7$.* □

It rests to determine which of these matrices are extremal.

4.5 Extremality

Let A and $u^1, \dots, u^6$ be as in Lemma 4.5. We shall investigate whether A is extremal by determining the solution space of the linear system on $B \in \mathcal{S}^6$ in Theorem 3.11.

There are 19 linear relations generated by the conditions $(Bu^j)_{\operatorname{supp} u^j} = 0$, $j = 1, \dots, 6$. In order for A to be extremal we must, however, have 20 linearly independent conditions $(Bu^j)_i = 0$ for index pairs (i, j) such that $(Au^j)_i = 0$. Hence there must be at least one such index pair with $i \notin \operatorname{supp} u^j$. By Lemma 4.5 this can only be $(Au^2)_6 = (Au^5)_4 = 0$ or $(Au^3)_6 = (Au^5)_2 = 0$. These relations are equivalent to the equalities $\phi_6 + \phi_9 = \pi + \phi_2$ and $\phi_7 = \phi_3 + \phi_4 + \phi_6$, respectively, and are related by the symmetry $(123456) \mapsto (543216)$ of the index set $\{1, \dots, 6\}$.

By possibly applying this symmetry we may without loss of generality assume that $\phi_7 - \phi_3 - \phi_4 - \phi_6 \geq 0$ and $\phi_6 + \phi_9 = \pi + \phi_2$. Then $A_{46} = \cos(\phi_6 - \phi_2)$. We shall consider the cases $\phi_7 - \phi_3 - \phi_4 - \phi_6 > 0$ and $\phi_7 - \phi_3 - \phi_4 - \phi_6 = 0$ separately.

Case $\phi_7 - \phi_3 - \phi_4 - \phi_6 > 0$: We have 21 linear relations on B. Consider how the conditions $(Bu^i)_j = 0$ coming from the zeros $u^1, \dots, u^5$ determine the elements of B. We shall use the method presented in Section 3.6. Set

$$F = \begin{pmatrix} 1 & 0 \\ -\cos\phi_1 & -\sin\phi_1 \\ \cos(\phi_1+\phi_2) & \sin(\phi_1+\phi_2) \\ -\cos(\phi_1+\phi_2+\phi_3) & -\sin(\phi_1+\phi_2+\phi_3) \\ \cos(\phi_1+\phi_2+\phi_3+\phi_4) & \sin(\phi_1+\phi_2+\phi_3+\phi_4) \\ -\cos(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5) & -\sin(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5) \\ -\cos(\phi_1+\phi_2-\phi_6) & -\sin(\phi_1+\phi_2-\phi_6) \end{pmatrix}.$$

Then we have

$$FPF^T = \begin{pmatrix} B_{33} & B_{34} & B_{35} & \star & \star & \star & \star \\ B_{34} & B_{44} & B_{45} & B_{14} & \star & \star & B_{46} \\ B_{35} & B_{45} & B_{55} & B_{15} & B_{25} & \star & B_{56} \\ \star & B_{14} & B_{15} & B_{11} & B_{12} & B_{13} & B_{16} \\ \star & \star & B_{25} & B_{12} & B_{22} & B_{23} & \star \\ \star & \star & \star & B_{13} & B_{23} & B_{33} & \star \\ \star & B_{46} & B_{56} & B_{16} & \star & \star & B_{66} \end{pmatrix}$$

for an appropriately chosen matrix $P \in \mathcal{S}^2$. Hence all elements of B except B_{24}, B_{26}, B_{36} are expressed as linear functions of P with one constraint on P coming from the double representation of B_{33}. This constraint is the relation $(FPF^T)_{11} = (FPF^T)_{66}$ and can equivalently be written as

$$\sin(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5)(P_{11}-P_{22}) - 2\cos(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5)P_{12} = 0.$$

The solution space of this equation is two-dimensional, with linearly independent solutions

$$P^1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad P^2 = \begin{pmatrix} \cos(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5) & \sin(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5) \\ \sin(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5) & -\cos(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5) \end{pmatrix}. \tag{5}$$

Here the solution P^1 corresponds to $B = A$.

By Lemma 4.2 the remaining relations $(Bu^6)_{\operatorname{supp} u^6} = 0$ on the still undetermined elements B_{24}, B_{26}, B_{36} are compatible if and only if

$$B_{22}u_{62}^2 + 2B_{23}u_{62}u_{63} + B_{33}u_{63}^2 = B_{44}u_{64}^2 + 2B_{46}u_{64}u_{66} + B_{66}u_{66}^2. \tag{6}$$

In this case these elements are determined uniquely by P.

It follows that for given $\phi_1, \dots, \phi_6$ the zero u^6 has to satisfy the relation

$$u_{62}^2 - 2\cos\phi_5 u_{62}u_{63} + u_{63}^2 = u_{64}^2 + 2\cos(\phi_6-\phi_2)u_{64}u_{66} + u_{66}^2. \tag{7}$$

This ensures the existence of the solution $B = A$. A second linearly independent solution exists if and only if in addition the relation

$$\begin{aligned} &\cos(\phi_1+\phi_2+\phi_3+\phi_4-\phi_5)u_{62}^2 - 2\cos(\phi_1+\phi_2+\phi_3+\phi_4)u_{62}u_{63} + \cos(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5)u_{63}^2 = \\ &= \cos(\phi_1-\phi_2-\phi_3-\phi_4-\phi_5)u_{64}^2 + 2\cos(\phi_1-\phi_3-\phi_4-\phi_5-\phi_6)u_{64}u_{66} + \cos(\phi_1+\phi_2-\phi_3-\phi_4-\phi_5-2\phi_6)u_{66}^2 \end{aligned} \tag{8}$$

is satisfied. In this case A is not extremal.

Case $\phi_3+\phi_4+\phi_6 = \phi_7$*:* Then we have the additional relations $(Bu^5)_2 = (Bu^3)_6 = 0$. These are equivalent to the relation $(FPF^T)_{57} = B_{26}$, with F defined as above and P being a linear combination of the solutions (5).

By Lemma 4.3 the remaining relations $(Bu^6)_{\operatorname{supp} u^6} = 0$ on the still undetermined elements B_{24}, B_{36} are compatible if and only if in addition to (6) the condition

$$B_{22}u_{62}^2 + 2B_{26}u_{62}u_{66} + B_{66}u_{66}^2 = B_{33}u_{63}^2 + 2B_{34}u_{63}u_{64} + B_{44}u_{64}^2$$

holds. In this case these elements are determined uniquely by P.

It follows that for given $\phi_1, \dots, \phi_6$ the zero u^6 has to satisfy the relations (7) and

$$u_{62}^2 - 2\cos(\phi_3+\phi_4-\phi_6)u_{62}u_{66} + u_{66}^2 = u_{63}^2 - 2\cos\phi_1 u_{63}u_{64} + u_{64}^2.$$

This ensures the existence of the solution $B = A$. A second linearly independent solution exists if and only if in addition the relations (8) and

$$\begin{aligned} &\cos(\phi_1+\phi_2+\phi_3+\phi_4-\phi_5)u_{62}^2 - 2\cos(\phi_1+\phi_2-\phi_5-\phi_6)u_{62}u_{66} + \cos(\phi_1+\phi_2-\phi_3-\phi_4-\phi_5-2\phi_6)u_{66}^2 = \\ &= \cos(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5)u_{63}^2 - 2\cos(\phi_2+\phi_3+\phi_4+\phi_5)u_{63}u_{64} + \cos(\phi_1-\phi_2-\phi_3-\phi_4-\phi_5)u_{64}^2 \end{aligned} \tag{9}$$

are satisfied. In this case A is not extremal.

4.6 Result

Let us summarize our findings. We have proven the following result, which exhaustively describes the sought exceptional extremal matrices.

Theorem 4.8. *The exceptional extremal matrices $A \in \mathcal{COP}^6$ with minimal zero support set 19 of Table 1 and with unit diagonal are given by*

(i) all matrices (1) *with* $\phi_i \in (0,\pi)$, $\phi_1+\cdots+\phi_5 < \pi$, $\phi_9 = \pi+\phi_2-\phi_6$, $\phi_3+\phi_4+\phi_6 < \phi_7$, $A_{\{2,3,4\}} \succ 0$, $A_{\{2,3,4,6\}}u = 0$ *for some* $u = (u_{62}, u_{63}, u_{64}, u_{66})^T \in \mathbb{R}^4_{++}$, *except those satisfying* (8)*;*

(ii) all matrices (1) *with* $\phi_i \in (0,\pi)$, $\phi_1+\cdots+\phi_5 < \pi$, $\phi_9 = \pi+\phi_2-\phi_6$, $\phi_3+\phi_4+\phi_6 = \phi_7$, $A_{\{2,3,4\}} \succ 0$, $A_{\{2,3,4,6\}}u = 0$ *for some* $u = (u_{62}, u_{63}, u_{64}, u_{66})^T \in \mathbb{R}^4_{++}$, *except those satisfying simultaneously* (8) *and* (9)*;*

(iii) the images of the matrices listed in (i) under the symmetry $(123456) \mapsto (543216)$. □

The matrices in (i) have 8 free parameters, namely the angles $\phi_1, \ldots, \phi_6$ and the 4 non-zero elements of u^6, constrained by (7) and a normalizing constraint, e.g., $||u^6|| = 1$. The matrices in (i)) have one parameter less due to the additional equality condition $\phi_3 + \phi_4 + \phi_6 = \phi_7$. However, there still remains the question whether such matrices actually exist. We shall answer this question in the affirmative by giving examples.

A matrix satisfying the conditions in (i) of the theorem is given by

$$\begin{pmatrix} 1 & -\frac{\sqrt{3}}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & 1 & -\frac{\sqrt{3}}{2} & A_{24} & \frac{1}{2} & \frac{\sqrt{2}}{2} \\ \frac{1}{2} & -\frac{\sqrt{3}}{2} & 1 & -\frac{\sqrt{3}}{2} & \frac{1}{2} & -\sqrt{\frac{1}{2}+\frac{\sqrt{2}}{4}} \\ \frac{1}{2} & A_{24} & -\frac{\sqrt{3}}{2} & 1 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{\sqrt{3}}{2} & 1 & -\frac{1}{2} \\ 0 & \frac{\sqrt{2}}{2} & -\sqrt{\frac{1}{2}+\frac{\sqrt{2}}{4}} & \frac{\sqrt{3}}{2} & -\frac{1}{2} & 1 \end{pmatrix},$$

$$A_{24} = \frac{(3+\sqrt{6})(2+\sqrt{2})(1-\sqrt{\frac{1}{2}+\frac{\sqrt{2}}{4}}) - \sqrt{2(7\sqrt{2}+6\sqrt{3})(7+5\sqrt{2}) - 2(39+27\sqrt{2}+22\sqrt{3}+16\sqrt{6})\sqrt{2+\sqrt{2}}}}{2},$$

corresponding to the choice $\phi_1 = \phi_2 = \phi_3 = \phi_4 = \phi_5 = \frac{\pi}{6}$, $\phi_6 = \frac{\pi}{3}$, $\phi_7 = \frac{3\pi}{4}$, $\phi_8 = \frac{\pi}{8}$, $\phi_9 = \frac{5\pi}{6}$.

A matrix satisfying the conditions in (ii) of the theorem is given by

$$\begin{pmatrix} 1 & -\frac{\sqrt{3}}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & 1 & -\frac{\sqrt{3}}{2} & A_{24} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{\sqrt{3}}{2} & 1 & -\frac{\sqrt{3}}{2} & \frac{1}{2} & -\frac{\sqrt{5}+1}{4} \\ \frac{1}{2} & A_{24} & -\frac{\sqrt{3}}{2} & 1 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{\sqrt{3}}{2} & 1 & -\frac{1}{2} \\ 0 & \frac{1}{2} & -\frac{\sqrt{5}+1}{4} & \frac{\sqrt{3}}{2} & -\frac{1}{2} & 1 \end{pmatrix},$$

$$A_{24} = \frac{(3+\sqrt{3})(3-\sqrt{5}) - 2\sqrt{2+6\sqrt{3}-2\sqrt{5}-2\sqrt{15}}}{2(5-\sqrt{5})},$$

corresponding to the choice $\phi_1 = \phi_2 = \phi_3 = \phi_4 = \phi_5 = \frac{\pi}{6}$, $\phi_6 = \frac{\pi}{3}$, $\phi_7 = \frac{2\pi}{3}$, $\phi_8 = \frac{\pi}{5}$, $\phi_9 = \frac{5\pi}{6}$.

5 Classification

In this section we present our classification of the extreme rays of the cone $\mathcal{COP}^6$. In addition to the extremal matrices listed in Section 2, there are manifolds of exceptional extremal matrices corresponding to the first 19 minimal zero support sets in Table 1.

The general form of an extremal matrix is given by $DPAP^TD$, where D is a positive definite diagonal matrix, P is a permutation matrix, and A is a matrix with unit diagonal which depends on a number of angles ϕ_i. Only the expressions for the factor A are given in the list below. Along with the expression of the matrix A we provide the set in which the angles ϕ_i vary.

In some cases the set of angles contains parts of its boundary, which manifests itself in the non-strictness of some of the inequalities defining this set. The reason is that some of the inequalities $(Au^i)_j \geq 0$ may become equalities without the appearance of an additional minimal zero.

Case NE

The non-exceptional extreme rays are generated by products $DPAP^TD$ with central factor $A = E_{11}, E_{12}, aa^T$, where a is one of the columns of the matrix

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

Case O5

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 0 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_5) & 0 \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & 0 \\ \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & 0 \\ -\cos\phi_5 & \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

where either $\phi_1 = \cdots = \phi_5 = 0$, or $\phi_i > 0$ for $i = 1, \ldots, 5$ and $\sum_{i=1}^5 \phi_i < \pi$.

Case 1

$$\begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & \cos\phi_2 \\ -1 & 1 & 1 & 1 & \cos\phi_2 & -1 \\ -1 & 1 & 1 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) \\ 1 & -1 & \cos\phi_2 & -\cos\phi_1 & 1 & -\cos\phi_2 \\ 1 & \cos\phi_2 & -1 & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 + \phi_2 < \pi$.

Case 2

$$\begin{pmatrix} 1 & -1 & -1 & -1 & 1 & \cos\phi_2 \\ -1 & 1 & 1 & 1 & -1 & \cos\phi_1 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_2 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_3 \\ 1 & -1 & \cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_3) & 1 & -\cos\phi_1 \\ \cos\phi_2 & \cos\phi_1 & -\cos\phi_2 & -\cos\phi_3 & -\cos\phi_1 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_2 < \phi_3 < \pi - \phi_1$.

Case 3

$$\begin{pmatrix} 1 & -1 & -1 & -1 & -\cos(\phi_1+\phi_2) & \cos\phi_4 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_2 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_3 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_4) & -\cos\phi_4 \\ -\cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_3) & \cos(\phi_1+\phi_4) & 1 & -\cos\phi_1 \\ \cos\phi_4 & -\cos\phi_2 & -\cos\phi_3 & -\cos\phi_4 & -\cos\phi_1 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_4 < \phi_3 < \phi_2 < \pi - \phi_1$.

Case 4

$$\begin{pmatrix} 1 & -1 & -1 & 1 & \cos(\phi_3+\phi_4) & -\cos\phi_4 \\ -1 & 1 & 1 & -1 & \cos\phi_2 & \cos\phi_4 \\ -1 & 1 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos\phi_4 \\ 1 & -1 & -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) \\ \cos(\phi_3+\phi_4) & \cos\phi_2 & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 \\ -\cos\phi_4 & \cos\phi_4 & \cos\phi_4 & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 + \phi_2 + \phi_3 + \phi_4 < \pi$.

Case 5

$$\begin{pmatrix} 1 & -1 & -1 & \cos(\phi_2+\phi_5) & -\cos\phi_5 & \cos\phi_3 \\ -1 & 1 & 1 & \cos(\phi_1+\phi_4) & \cos\phi_5 & -\cos\phi_4 \\ -1 & 1 & 1 & \cos(\phi_1+\phi_3) & \cos\phi_5 & -\cos\phi_3 \\ \cos(\phi_2+\phi_5) & \cos(\phi_1+\phi_4) & \cos(\phi_1+\phi_3) & 1 & -\cos\phi_2 & -\cos\phi_1 \\ -\cos\phi_5 & \cos\phi_5 & \cos\phi_5 & -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) \\ \cos\phi_3 & -\cos\phi_4 & -\cos\phi_3 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1+\phi_2+\phi_4+\phi_5 < \pi, \phi_3 < \phi_4$.

Case 6

$$\begin{pmatrix} 1 & -1 & -1 & \cos\phi_2 & \cos\phi_1 & \cos\phi_5 \\ -1 & 1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) \\ -1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_1 & -\cos\phi_5 \\ \cos\phi_2 & -\cos\phi_2 & \cos(\phi_1+\phi_3) & 1 & -\cos\phi_3 & -\cos\phi_4 \\ \cos\phi_1 & \cos(\phi_2+\phi_3) & -\cos\phi_1 & -\cos\phi_3 & 1 & \cos(\phi_1+\phi_5) \\ \cos\phi_5 & \cos(\phi_2+\phi_4) & -\cos\phi_5 & -\cos\phi_4 & \cos(\phi_1+\phi_5) & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1+\phi_3+\phi_5 < \phi_4, \phi_2+\phi_4+\phi_5 < \pi$.

Case 7

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos\phi_4 & -1 & \cos\phi_1 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos\phi_1 & -1 \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & \cos\phi_2 \\ \cos\phi_4 & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) \\ -1 & \cos\phi_1 & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & -\cos\phi_5 \\ \cos\phi_1 & -1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 \le \phi_5, \phi_2+\phi_3+\phi_4+\phi_5 < \pi, \phi_1+\phi_5 \neq \pi$.

Case 8

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & \cos\phi_5 \\ -1 & 1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & \cos(\phi_5+\phi_6) & -\cos\phi_5 \\ -\cos\phi_2 & \cos\phi_2 & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_1+\phi_4) \\ \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_1 & 1 & \cos(\phi_1-\phi_3) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_3 & \cos(\phi_1-\phi_3) & 1 & -\cos\phi_6 \\ \cos\phi_5 & -\cos\phi_5 & \cos(\phi_1+\phi_4) & -\cos\phi_4 & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_3+\phi_4 \le \phi_1+\phi_6, \phi_2+\phi_3+\phi_5+\phi_6 \le \pi, \phi_1+\phi_4 < \phi_3+\phi_6$ with either $\phi_2+\phi_3 \neq \phi_5+\phi_6$ or with $\phi_2+\phi_3 = \phi_5+\phi_6 = \frac{\pi}{2}$ or with $\phi_2+\phi_3 = \phi_5+\phi_6, \phi_1+\phi_6 = \phi_3+\phi_4$.

Case 9.1

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & \cos\phi_5 \\ -1 & 1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & \cos(\phi_5-\phi_6) & -\cos\phi_5 \\ -\cos\phi_2 & \cos\phi_2 & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_1+\phi_4) \\ \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_1 & 1 & \cos(\phi_4+\phi_6) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & \cos(\phi_5-\phi_6) & -\cos\phi_3 & \cos(\phi_4+\phi_6) & 1 & -\cos\phi_6 \\ \cos\phi_5 & -\cos\phi_5 & cos(\phi_1+\phi_4) & -\cos\phi_4 & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_2+\phi_3 < \pi, \phi_2+\phi_3+\phi_5 < \pi+\phi_6, \phi_1+\phi_4+\phi_6 < \phi_3$, $\phi_2+\phi_3+\phi_6 < \pi+\phi_5$, excluding $\phi_2+\phi_3+\phi_6 = \phi_5$.

Case 9.2

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & \cos\phi_5 \\ -1 & 1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & -\cos(\phi_2+\phi_3) & -\cos\phi_5 \\ -\cos\phi_2 & \cos\phi_2 & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_1+\phi_4) \\ \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_1 & 1 & \cos(\phi_4+\phi_6) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & -\cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_4+\phi_6) & 1 & -\cos\phi_6 \\ \cos\phi_5 & -\cos\phi_5 & \cos(\phi_1+\phi_4) & -\cos\phi_4 & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_2+\phi_3 < \pi, \phi_2+\phi_3+\phi_5 < \pi+\phi_6, \phi_1+\phi_4+\phi_6 < \phi_3$, $\phi_2+\phi_3+\phi_6 > \pi+\phi_5$.

Case 10

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & \cos\phi_5 \\ -1 & 1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & \cos(\phi_5-\phi_6) & -\cos\phi_5 \\ -\cos\phi_2 & \cos\phi_2 & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_3+\phi_6) \\ \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_1 & 1 & \cos(\phi_4+\phi_6) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & \cos(\phi_5-\phi_6) & -\cos\phi_3 & \cos(\phi_4+\phi_6) & 1 & -\cos\phi_6 \\ \cos\phi_5 & -\cos\phi_5 & \cos(\phi_3+\phi_6) & -\cos\phi_4 & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 + \phi_2 + \phi_4 + \phi_5 < \pi, \phi_3 + \phi_4 + \phi_6 < \phi_1,\ \phi_2 + \phi_3 + \phi_6 \neq \phi_5$.

Case 11

$$\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_6) & \cos(\phi_1+\phi_4) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_6 & \cos(\phi_3+\phi_5) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_4+\phi_5) & -\cos(\phi_1+\phi_2+\phi_6) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_4+\phi_5) & 1 & \cos(\phi_3-\phi_6) & -\cos\phi_5 \\ \cos(\phi_2+\phi_6) & -\cos\phi_6 & -\cos(\phi_1+\phi_2+\phi_6) & \cos(\phi_3-\phi_6) & 1 & b_3 \\ \cos(\phi_1+\phi_4) & \cos(\phi_3+\phi_5) & -\cos\phi_4 & -\cos\phi_5 & b_3 & 1 \end{pmatrix},$$

$b_3 = \frac{-\cos(\phi_3-\phi_6)\sin(\phi_4)+\cos(\phi_1+\phi_2+\phi_6)\sin(\phi_5)}{\sin(\phi_4+\phi_5)}$, $\phi_i > 0, \phi_1+\phi_2+\phi_3+\phi_4+\phi_5 < \pi, \pi-\phi_1-\phi_4-\phi_5+\phi_3-\phi_2 < 2\phi_6 < \pi-\phi_1+\phi_5+\phi_3+\phi_4-\phi_2$.

Case 12

$$\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_4 & \cos(\phi_3+\phi_6) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & b_1 & \cos(\phi_5+\phi_7) & -\cos\phi_5 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & b_1 & 1 & \cos(\phi_3-\phi_4) & -\cos\phi_6 \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & \cos(\phi_5+\phi_7) & \cos(\phi_3-\phi_4) & 1 & -\cos\phi_7 \\ \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_6) & -\cos\phi_5 & -\cos\phi_6 & -\cos\phi_7 & 1 \end{pmatrix},$$

$b_1 = \frac{\sin(\phi_5+\phi_7)\cos\phi_6-\cos(\phi_3-\phi_4)\sin\phi_5}{\sin\phi_7}$, $\phi_i > 0, \phi_1+\phi_2+\phi_4+\phi_5+\phi_7 < \pi, \phi_4+\phi_7 > \phi_3+\phi_6, \phi_4+\phi_6 > \phi_3+\phi_7, \phi_7+\phi_3+\phi_6 > \phi_4$.

Case 13.1

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & -\cos(\phi_1+\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_6 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & -\cos(\phi_2+\phi_3+\phi_4) & \cos(\phi_1+\phi_6) \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & -\cos(\phi_3+\phi_4+\phi_5) \\ -\cos(\phi_1+\phi_2+\phi_3) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) \\ \cos(\phi_5+\phi_6) & -\cos(\phi_2+\phi_3+\phi_4) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & -\cos\phi_5 \\ -\cos\phi_6 & \cos(\phi_1+\phi_6) & -\cos(\phi_3+\phi_4+\phi_5) & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 \end{pmatrix},$$

$\phi_i > 0, \sum_{j=1}^{6}\phi_j < 2\pi, \phi_i+\phi_{i+1} < \pi, i = 1,\ldots,5, \phi_1+\phi_6 < \pi, \phi_1+\phi_2+\phi_3 \geq \phi_4+\phi_5+\phi_6, \phi_2+\phi_3+\phi_4 \geq \phi_1+\phi_5+\phi_6, \phi_3+\phi_4+\phi_5 \geq \phi_1+\phi_2+\phi_6$, such that $\sum_{j=1}^{6}\phi_j \neq \pi$, or at least two of the non-strict inequalities are equalities.

Case 13.2

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & -\cos(\phi_1+\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_6 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & -\cos(\phi_1+\phi_5+\phi_6) & \cos(\phi_1+\phi_6) \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & -\cos(\phi_3+\phi_4+\phi_5) \\ -\cos(\phi_1+\phi_2+\phi_3) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) \\ \cos(\phi_5+\phi_6) & -\cos(\phi_1+\phi_5+\phi_6) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & -\cos\phi_5 \\ -\cos\phi_6 & \cos(\phi_1+\phi_6) & -\cos(\phi_3+\phi_4+\phi_5) & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 \end{pmatrix},$$

$\phi_i > 0, \sum_{j=1}^{6}\phi_j < 2\pi, \phi_i+\phi_{i+1} < \pi, i = 1,\ldots,5, \phi_1+\phi_6 < \pi, \phi_1+\phi_2+\phi_3 \geq \phi_4+\phi_5+\phi_6, \phi_2+\phi_3+\phi_4 \leq \phi_1+\phi_5+\phi_6, \phi_3+\phi_4+\phi_5 \geq \phi_1+\phi_2+\phi_6$, such that $\sum_{j=1}^{6}\phi_j \neq \pi$, or at least two of the non-strict inequalities are equalities.

Case 14

$$\begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 \end{pmatrix}.$$

Case 15

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_4) \\ -1 & 1 & \cos\phi_2 & \cos\phi_1 & \cos(\phi_5+\phi_6) & -\cos\phi_6 \\ -\cos\phi_2 & \cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & \cos(\phi_3+\phi_5) \\ -\cos\phi_1 & \cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_4+\phi_5) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_3 & \cos(\phi_4+\phi_5) & 1 & -\cos\phi_5 \\ \cos(\phi_1+\phi_4) & -\cos\phi_6 & \cos(\phi_3+\phi_5) & -\cos\phi_4 & -\cos\phi_5 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1+\phi_2+\phi_3+\phi_4+\phi_5 < \pi, \phi_2+\phi_3+\phi_5+\phi_6 \leq \pi, \phi_6 \geq \phi_1+\phi_4$.

Case 16

$$\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_4 & \cos(\phi_3+\phi_6) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_5+\phi_6) & \cos(\phi_5+\phi_7) & -\cos\phi_5 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_5+\phi_6) & 1 & \cos(\phi_6-\phi_7) & -\cos\phi_6 \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & \cos(\phi_5+\phi_7) & \cos(\phi_6-\phi_7) & 1 & -\cos\phi_7 \\ \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_6) & -\cos\phi_5 & -\cos\phi_6 & -\cos\phi_7 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1+\phi_2+\phi_4+\phi_5+\phi_7 \le \pi, \phi_4+\phi_7 > \phi_3+\phi_6,\ \phi_4+\phi_6 \ge \phi_3+\phi_7$.

Case 17

$$\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_4 & \cos(\phi_3+\phi_6) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_5-\phi_6) & \cos(\phi_5+\phi_7) & -\cos\phi_5 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_5-\phi_6) & 1 & \cos(\phi_6+\phi_7) & -\cos\phi_6 \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & \cos(\phi_5+\phi_7) & \cos(\phi_6+\phi_7) & 1 & -\cos\phi_7 \\ \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_6) & -\cos\phi_5 & -\cos\phi_6 & -\cos\phi_7 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_3+\phi_6+\phi_7 < \phi_4, \phi_1+\phi_5+\phi_7+\phi_2+\phi_4 < \pi$.

Case 18

$$\begin{pmatrix} 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & -\cos(\phi_3+\phi_6) \\ -\cos\phi_4 & 1 & -\cos\phi_5 & \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_4) & \cos(\phi_3+\phi_4+\phi_6) \\ \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_2-\phi_6) \\ \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_5) & -\cos\phi_1 & 1 & -\cos\phi_2 & -\cos(\phi_2-\phi_6) \\ -\cos\phi_3 & \cos(\phi_3+\phi_4) & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & \cos\phi_6 \\ -\cos(\phi_3+\phi_6) & \cos(\phi_3+\phi_4+\phi_6) & \cos(\phi_1+\phi_2-\phi_6) & -\cos(\phi_2-\phi_6) & \cos\phi_6 & 1 \end{pmatrix},$$

$\phi_1, \dots, \phi_5 > 0, \phi_1+\phi_2+\phi_3+\phi_4+\phi_5 < \pi, -\phi_3 < \phi_6 < \phi_2$.

Case 19

$$\begin{pmatrix} 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_3+\phi_6) \\ -\cos\phi_4 & 1 & -\cos\phi_5 & a_{24} & \cos(\phi_3+\phi_4) & -\cos\phi_7 \\ \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & a_{36} \\ \cos(\phi_2+\phi_3) & a_{24} & -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_6-\phi_2) \\ -\cos\phi_3 & \cos(\phi_3+\phi_4) & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_6 \\ \cos(\phi_3+\phi_6) & -\cos\phi_7 & a_{36} & \cos(\phi_6-\phi_2) & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i \in (0,\pi)$, $\phi_1+\phi_2+\phi_3+\phi_4+\phi_5 < \pi$, $\phi_2 < \phi_6$, $\phi_3+\phi_4+\phi_6 \le \phi_7$, $A_{\{2,3,4\}} \succ 0$, $A_{\{2,3,4,6\}}$ with positive kernel vector, excluding matrices satisfying $\phi_3+\phi_4+\phi_6 < \phi_7$ and (8) or $\phi_3+\phi_4+\phi_6 = \phi_7$ and (8) and (9).

We are now ready to formulate our main result.

Theorem 5.1. *Let the matrix C generate an extreme ray of $\mathcal{COP}^6$. Then there exists a permutation matrix $P \in S_6$, a positive definite diagonal matrix D, and a matrix A given by one of the above forms NE, O5, or 1–19 with the parameters ϕ_i in the corresponding range, such that $C = P^T DADP$.*

On the other hand, every matrix product of this form generates an extreme ray of $\mathcal{COP}^6$. □

6 Conclusion

In this contribution we classified the extreme rays of the 6×6 copositive cone. The set of these extreme rays is a stratified real algebraic manifold.

The classification proceeds via an intermediate classification of the minimal zero support set of the matrix generating the extreme ray. This set is a discrete object. It turns out that different strata of the manifold of extreme rays may correspond to the same minimal zero support set, and hence this object is too coarse to classify the strata. However, the strata can be distinguished by the additional information which of the inequalities $(Au^i)_j \ge 0$ are equalities and which are strict. As a rule, strata corresponding to the same support set have different dimensions, and the one with smaller dimension lies on the boundary of the one with larger dimension. There may be, however, also non-isomorphic (with respect to permutation of the indices) strata of the same dimension corresponding to the same support set.

In Table 7 below we present the dimensions of the mutually non-isomorphic strata of exceptional extremal matrices with unit diagonal corresponding to the minimal zero support sets 1–19 in Table 1. The respective maximal dimension equals the number of free parameters in the expressions for the factor A given in

Section 5. The strata of smaller dimension are obtained by letting some of the non-strict inequalities on the parameters be equalities. Removing the restriction that the diagonal elements of the matrix equal 1 increases all dimensions by 6.

Another observation is that the dimension of a stratum does not necessarily drop if a minimal zero support is added to the support set. The dimensions of the maximal strata in cases 12 and 16 of Table 1 are equal, despite the fact that one of the support sets strictly contains the other. This can be explained by the equality $(Au^2)_5 = 0$ in case 12, which in case 16 is a strict inequality.

There are strata which contain "holes" carved out by embedded submanifolds of non-extremal matrices, a phenomenon which does not occur for lower order of the copositive cone. These submanifolds may have a co-dimension strictly larger than 1, as is the case for the manifold described by (ii) of Theorem 4.8.

In the case of 6×6 matrices new phenomena appear which are not present at lower orders. In particular, the minimal zero support set may not cover all off-diagonal entries, which leads to elements b_i in the parameterized matrix which are a priori not part of a degenerated PSD submatrix A_I corresponding to a minimal zero support I. The first order conditions $Au \geq 0$ at the minimal zeros yield a system of non-strict inequalities on the b_i whose feasible set is a polyhedron. In order to further constrain the values of these variables to extremal points of the polyhedron we have to use the condition that A is extremal. Thus we do not classify the reduced matrices and check for extremality a posteriori, as in [16].

We obtained also directly new constraints on the minimal zero support set of an extremal copositive matrix. For instance, the combination of supports appearing in cases 43 or 44 of Table 1, augmented with an appropriate number of zero entries, cannot occur at any order, because the resulting first order constraints are incompatible. Another set of constraints can be obtained from the results in Section 3.2, which link minimal zero supports to linear dependence of the corresponding minimal zeros.

The number of isomorphism classes of strata of extremal matrices is an order of magnitude larger than in the case of 5×5 copositive matrices, which suggests that the complexity of the copositive cone very rapidly increases with its order. The picture can be made more accessible by the following notion.

Definition 6.1. Let $\mathcal{M}_n$ be the stratified real algebraic manifold of extreme rays of the copositive cone $\mathcal{COP}^n$. A stratum $\mathcal{S}$ of $\mathcal{M}_n$ is called *essential* if there does not exist a stratum $\mathcal{S}' \neq \mathcal{S}$ such that $\mathcal{S} \subset \partial\mathcal{S}'$.

Clearly the stratum of dimension 14 corresponding to case 19 in Table 1 is essential, because no other stratum has larger dimension. Is there any other essential stratum?

In [17] necessary conditions on the minimal zero support set of an exceptional extremal matrix of $\mathcal{COP}^n$ have been found. How can these conditions be tightened using the additional condition that the matrix lies on an essential stratum?

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No.	No. in [17]	$\operatorname{supp} \mathcal{V}^A_{\min}$	result
1	2	{1,2},{1,3},{1,4},{2,5},{3,6},{4,5,6}	exceptional extremal
2	3	{1,2},{1,3},{1,4},{2,5},{3,5,6},{4,5,6}	matrices with this
3	4	{1,2},{1,3},{1,4},{2,5,6},{3,5,6},{4,5,6}	minimal zero support
4	5	{1,2},{1,3},{2,4},{3,4,5},{1,5,6},{4,5,6}	set exist
5	6	{1,2},{1,3},{1,4,5},{2,4,6},{3,4,6},{4,5,6}	
6	8	{1,2},{1,3},{2,4,5},{3,4,5},{2,4,6},{3,5,6}	
7	9	{1,5},{2,6},{1,2,3},{2,3,4},{3,4,5},{4,5,6}	
8	13	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{2,5,6}	
9	15	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{4,5,6}	
10	16	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,5,6},{4,5,6}	
11	21	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,6}	
12	22	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,5,6}	
13	34	{1,2,3},{2,3,4},{3,4,5},{4,5,6},{1,5,6},{1,2,6}	
14	36	{1,2},{1,3},{1,4},{2,5},{4,5},{3,6},{5,6}	
15	37	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6},{4,5,6}	
16	41	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,6},{3,5,6}	
17	42	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,5,6},{4,5,6}	
18	43	{1,2,3},{2,3,4},{3,4,5},{1,4,5},{1,2,5},{3,4,6},{1,4,6},{1,2,6}	
19	23	{3,4,5},{1,4,5},{1,2,5},{1,2,3},{1,5,6},{2,3,4,6}	
20	1	{1,2},{1,3},{1,4},{2,5},{3,6},{5,6}	copositivity and
21	11	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6}	extremality enforce
22	12	{1,2},{2,3,4},{3,4,5},{4,5,6},{2,5,6},{2,3,6}	additional minimal
23	17	{1,2},{1,3,4},{2,3,5},{3,4,5},{2,4,6},{3,4,6}	zero supports
24	24	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{3,4,6},{3,5,6}	
25	25	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{3,4,6},{4,5,6}	
26	28	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,4,5},{2,3,6}	
27	30	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,4,6},{3,5,6}	
28	32	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{1,5,6},{4,5,6}	
29	39	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6},{3,5,6}	
30	7	{1,2},{1,3},{2,4,5},{3,4,5},{2,4,6},{3,4,6}	linear span of
31	10	{1,2},{1,3,4},{1,3,5},{2,3,6},{3,4,6},{3,5,6}	minimal zeros is
32	14	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{3,5,6}	a proper subspace
33	18	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{1,5,6}	
34	19	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6}	
35	20	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{3,5,6}	
36	26	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{2,4,6}	
37	27	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{3,4,6}	
38	38	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{2,5,6},{3,5,6}	
39	40	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{3,5,6},{4,5,6}	
40	44	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{2,4,6},{3,5,6},{4,5,6}	
41	35	{1,2,3,4},{2,3,4,5},{3,4,5,6},{1,4,5,6},{1,2,5,6},{1,2,3,6}	
42	33	{1,2,5},{1,4,5},{1,2,3},{3,4,5},{2,3,6},{3,4,6}	
43	31	{1,2,5},{1,4,5},{1,2,3},{3,4,5},{1,3,6},{3,5,6}	first order conditions
44	29	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{2,3,6},{2,5,6}	are incompatible

Table 1: Candidate minimal support sets $\mathcal{I}$ of exceptional extreme matrices in $\mathcal{COP}^6$

Case No.	location of the b_i	Case No.	location of the b_i
1	$b_1 = A_{26}$, $b_2 = A_{35}$	2	$b_1 = A_{16}$, $b_2 = A_{26}$
3	$b_1 = A_{15}$, $b_2 = A_{16}$	4	$b_1 = A_{25}$, $b_2 = A_{26}$, $b_3 = A_{36}$
5	$b_1 = A_{16}$, $b_2 = A_{25}$, $b_3 = A_{35}$	6	$b_1 = A_{14}$, $b_2 = A_{15}$, $b_3 = A_{16}$
7	$b_1 = A_{14}$, $b_2 = A_{25}$, $b_3 = A_{36}$, $b_4 = A_{16}$	8	$b_1 = A_{23}$, $b_2 = A_{16}$, $b_3 = A_{45}$
9,10	$b_1 = A_{23}$, $b_2 = A_{25}$, $b_3 = A_{16}$	11	$b_1 = A_{35}$, $b_2 = A_{45}$, $b_3 = A_{56}$
12	$b_1 = A_{34}$, $b_2 = A_{45}$	13	$b_1 = A_{14}$, $b_2 = A_{25}$, $b_3 = A_{36}$
15	$b_1 = A_{23}$, $b_2 = A_{24}$	16	$b_1 = A_{45}$
17	$b_1 = A_{34}$	18	$b_1 = A_{56}$

Table 2: Location of the variables b_i in the candidate matrices

Case No.	equalities	Case No.	equalities
1	$(Au^5)_5 = (Au^4)_6 = 0$	2	$(Au^2)_6 = (Au^4)_6 = 0$
3	$(Au^1)_5 = (Au^3)_6 = 0$	4	$(Au^3)_5 = (Au^1)_6 = (Au^2)_6 = 0$
5	$(Au^2)_6 = (Au^1)_5 = (Au^2)_5 = 0$	6	$(Au^1)_4 = (Au^2)_5 = (Au^2)_6 = 0$
7	$(Au^1)_4 = (Au^1)_2 = (Au^2)_3 = (Au^2)_1 = 0$	8	$(Au^1)_3 = (Au^1)_6 = (Au^2)_5 = 0$
9.1	$(Au^1)_3 = (Au^6)_2 = (Au^1)_6 = 0$	9.2	$(Au^1)_3 = (Au^1)_5 = (Au^1)_6 = 0$
10	$(Au^1)_3 = (Au^4)_5 = (Au^1)_6 = 0$	11	$(Au^1)_5 = (Au^2)_5 = (Au^6)_5 = 0$
12	$(Au^6)_4 = (Au^2)_5 = 0$	13.1	$(Au^1)_4 = (Au^2)_5 = (Au^3)_6 = 0$
13.2	$(Au^1)_4 = (Au^5)_2 = (Au^3)_6 = 0$	15	$(Au^1)_3 = (Au^1)_4 = 0$
16	$(Au^6)_5 = 0$	17	$(Au^6)_4 = 0$
18	$(Au^3)_6 = 0$	19	$(Au^2)_6 = (Au^5)_4 = 0$

Table 3: Equalities $(Au^j)_k = 0$ determining the variables b_i

Case No.	Generator(s)	Group	Inequalities
1	$(1,3,2,4,6,5)$	S_2	
2	$(1,2,4,3,5,6)$	S_2	$\phi_2 \leq \phi_3$
3	$(1,3,2,4,5,6); (1,2,4,3,5,6); (1,2,3,4,6,5)$	$S_3 \times S_2$	$\phi_4 \leq \phi_3 \leq \phi_2$
5	$(1,3,2,4,5,6)$	S_2	$\phi_3 \leq \phi_4$
6	$(1,3,2,5,4,6)$	S_2	$\phi_2 + \phi_4 + \phi_5 \leq \pi$
7	$(6,5,4,3,2,1)$	S_2	$\phi_1 \leq \phi_5$
8	$(2,1,6,4,5,3)$	S_2	$\phi_3 + \phi_4 \leq \phi_1 + \phi_6$
11	$(2,1,4,3,5,6)$	S_2	
13	$(6,5,4,3,2,1); (6,1,2,3,4,5)$	D_6	$\phi_1 + \phi_2 + \phi_3 \geq \phi_4 + \phi_5 + \phi_6$, $\phi_3 + \phi_4 + \phi_5 \geq \phi_1 + \phi_2 + \phi_6$
14	$(1,4,3,2,5,6); (5,2,6,4,1,3)$	S_2^2	
15	$(1,2,4,3,6,5)$	S_2	
16	$(3,6,1,4,5,2)$	S_2	$\phi_4 + \phi_6 \geq \phi_3 + \phi_7$
17	$(2,1,4,3,5,6)$	S_2	
18	$(1,2,3,4,6,5); (4,3,2,1,5,6)$	S_2^2	
19	$(5,4,3,2,1,6)$	S_2	$\phi_7 - \phi_3 - \phi_4 - \phi_6 \geq \phi_6 + \phi_9 - \pi - \phi_2$

Table 4: Symmetry groups, their generators, and enforced inequalities

Case No.	Index subset	Certifying vectors v
1	$\{2,3,4,5\}$	$e_3 - e_2$
2	$\{2,3,4,5\}, \{2,3,4,6\}$	$e_3 - e_2, e_2 + e_6$
3	$\{2,3,4,5\}, \{2,3,4,6\}$	$e_2 + e_5, e_2 + e_6$
4	$\{2,3,5,6\}$	$e_5 + e_6$
5	$\{2,3,4,5\}, \{2,3,5,6\}$	$e_3 - e_2, e_2 - e_3$
6	$\{1,4,5,6\}$	$e_4 + e_5$
7	$\{1,3,4,6\}$	$e_3 + e_4$
8	$\{1,4,5,6\}, \{2,3,4,5\}$	$e_4 + e_6$, $e_3 + e_4$ ($\phi_1 \leq 2\phi_3$) or $e_3 + e_5$ ($\phi_3 \leq 2\phi_1$)
9	$\{2,3,4,5\}, \{2,3,5,6\}$	$e_3 + e_4$, $e_5 + e_6$ (9.1) or $e_2 + e_6$ (9.2)
10	$\{2,3,4,5\}$	$e_3 + e_5$
11	$\{1,3,4,5\}, \{2,3,4,5\}$	$e_1 + e_3, e_2 + e_4$
	$\{1,4,5,6\}$	$\sin(\phi_6 - \phi_3)e_1 - \sin(\phi_2 + \phi_6)e_4 + \sin(\phi_2 + \phi_3)e_5$
	$\{2,3,5,6\}$	$\sin(\phi_1 + \phi_2 + \phi_6)e_2 - \sin\phi_6 e_3 + \sin(\phi_1 + \phi_2)e_5$
12	$\{1,3,4,5\}, \{2,3,4,5\}$	$e_1 + e_3, e_2 + e_4$
	$\{1,4,5,6\}$	$\sin(\phi_4 - \phi_3)e_1 - \sin(\phi_2 + \phi_4)e_4 + \sin(\phi_2 + \phi_3)e_5$
13	$\{1,2,4,5\}, \{1,3,4,6\}, \{2,3,5,6\}$	$e_4\cos\phi_4 + e_5$, $e_1 + e_6$, $e_2 + \cos\phi_2 e_3$
15	$\{2,3,4,5\}, \{2,3,4,6\}$	$e_3 + e_5, e_4 + e_6$
16	$\{1,4,5,6\}$	$e_5 + e_6$ ($2\phi_6 \geq \phi_7$) or $e_4\cos\phi_6 + e_6$ ($\phi_6 \leq \phi_7$)
	$\{1,3,4,5\}, \{2,3,4,5\}$	$e_1 + e_3, e_2 + e_4$
17	$\{1,3,4,5\}, \{2,3,4,5\}$	$e_1 + e_3$, $e_2 + e_4$
18	$\{1,3,5,6\}, \{2,3,5,6\}$	$e_1 + e_5$ ($-\phi_3 \leq 2\phi_6$) or $e_1 + e_6$ ($\phi_6 \leq \phi_3$), $e_2 + e_3$,
	$\{2,4,5,6\}$	$e_4 + e_5$ ($2\phi_6 \leq \phi_2$) or $e_4 + e_6$ ($-\phi_2 \leq \phi_6$)

Table 5: Copositivity certifying vectors for index subsets of cardinality 4

Case No.	Minimal zero support	Case No.	Minimal zero support
20	$\{4,5\}$ or $\{4,6\}$	21	$\{4,5,6\}$
22	$\{1,4,5\}$	23	$\{2,5,6\}$
24	$\{2,4,6\}$ or $\{2,5,6\}$	25	$\{1,5,6\}$ or $\{2,4,6\}$ or $\{2,5,6\}$
26	$\{2,4,6\}$	27	$\{2,4,6\}$
28	$\{1,2,6\}$	29	$\{4,5,6\}$

Table 6: Additionally appearing minimal zero support set

Case No.	Dim.	Case No.	Dim.	Case No.	Dim.	Case No.	Dim.
1	2	6	5	11	6	16	7,6,6,5
2	3	7	5,4	12	7	17	7
3	4	8	6,5,5,4	13	6,6,5,5,4,3	18	6
4	4	9	6,6	14	0	19	8,7
5	5	10	6	15	6,5,5		

Table 7: Dimensions of strata of extremal matrices with unit diagonal