The extreme rays of the 6×6 copositive cone

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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 to copositive matrices of arbitrary order.

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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, 20].

Verifying copositivity of a given matrix is a co-NP-complete problem [22], 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 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, 25, 4, 5, 24, 23].

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 [21].

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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 of the extreme rays of $\mathcal{COP}^6$.

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 $u = (u_1, \dots, u_n)^T \in \mathbb{R}^n_+$ is the subset of indices $j \in \{1, \dots, n\}$ 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 $2^{\{1,\dots,n\}}$, the power set of $\{1, \dots, n\}$. 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 subsets of the power set, up to a permutation of the indices. In Table 1 we reproduce this list up to permutations of the indices $1, \dots, 6$. We consider each of these support 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 support sets we determine all exceptional extremal matrices $A \in \mathcal{COP}^6$ which have the given 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 $\mathcal{I} \subset 2^{\{1,\dots,6\}}$. 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 support sets in Table 1. The most difficult case necessitates an individual approach, which will be presented in Section 4. Finally, we summarize our findings in Section 6, where we 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 (PSD) 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 write $A \succ 0$ for A being positive definite.

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 $\mathbf{0} = (0, \dots, 0)^T$ the all-zeros vector. Similarly we denote by $\mathbf{1} = (1, \dots, 1)^T$ 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 $I \subset \{1, \dots, n\}$ 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 $\mathcal{I} \subset 2^{\{1,\dots,n\}}$ be a support 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 $\operatorname{supp} u = \{i \in \{1, \dots, n\} \mid u_i \neq 0\}$. We also define $\operatorname{supp}_{\geq 0} u = \{i \in \{1, \dots, n\} \mid u_i \geq 0\}$.

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 $\operatorname{supp} \mathcal{V}^A_{\min}$. Up to multiplication of the minimal zeros by positive constants, these two sets are in bijective correspondence for any given copositive matrix A [17, Lemma 3.5].

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 $C \in \mathcal{M}$. Otherwise we shall call A *reducible* with respect to C or $\mathcal{M}$.

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}, $1 \leq i, j \leq 6$, 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 $DPAP^TD$, 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 method

Out of the 44 support sets in Table 1 there are two (cases 19 and 41) which contain supports of cardinality 4 and require a separate consideration. All other support 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. Several arguments will be illustrated by examples.

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. In this way $\mathcal{I}$ 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], A being extremal implies $A_{ij} \in [-1, 1]$ 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 the 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 $i, j \in \{1, \dots, n\}$. 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 diagonal $\mathbf{1}$ and suppose there exists a minimal zero u of A with support $\{i, j, k\}$, where $i, j, k \in \{1, \dots, n\}$ 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 $\lambda u_{\{i,j,k\}} = (\sin\phi_i, \sin\phi_j, \sin\phi_k)^T = (\sin\phi_i, \sin(\phi_i + \phi_k), \sin\phi_k)^T$.

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 equality relations on the angles which allow to express some of them by the others. However, in general this parameterizes only a part of the off-diagonal entries of the matrix A, in particular, those which are covered by the support 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 parameterizations are given in Section 5, with the location of the variables b_i in Table 2, if there are any.

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:

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

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

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

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

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

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

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

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

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

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

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

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

Along with the elements A_{ij} we 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 in general, they can be deduced from their supports and Lemmas 3.1, 3.3.

In Subsection 3.3 below we shall further constrain the set of possible extremal matrices with a given minimal zero support set by using additional conditions imposed by the copositivity of the matrix. However, first we shall consider special constellations of the support 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 irreducible with respect to the cone $\mathcal{S}_+^n$ if and only if* $\operatorname{span} \mathcal{V}_{\min}^A = \mathbb{R}^n$.

We now show that under some circumstances we may deduce the linear dependence of minimal zeros just from their supports. Suppose the minimal zero support set $\mathcal{V}_{\min}^A$ of a matrix $A \in \mathcal{COP}^n$ with diagonal $\mathbf{1}$ 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 submatrix 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 reducible 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 Table 3 we list the supports of the successively removed minimal zeros for these cases.

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.

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 Subsection 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 $(Au)_j \geq 0,\ j = 1,\dots,6$, 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 $\mathcal{I} \subset 2^{\{1,\dots,n\}}$ be a support set and let $A \in \mathcal{COP}^n$ be an exceptional extremal copositive matrix with diagonal $\mathbf{1}$ 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. 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 4 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 also necessary in order for A to be extremal, see below in Subsection 4.5.

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, happen that these constraints are incompatible. We first state the following auxiliary result. Suppose the minimal zero support set $\mathcal{V}^A_{\min}$ of an extremal matrix $A \in \mathcal{COP}^n$ with diagonal $\mathbf{1}$ has a subset of the form $\{\{a,b,c\},\{b,c,d\}\}$, where $I = \{a,b,c,d\}$ consists of 4 mutually distinct indices. Then by Lemma 3.3 the corresponding 4×4 submatrix 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 zero support set $\mathcal{V}^A_{\min}$ of a matrix $A \in \mathcal{COP}^n$ with diagonal* **1** *has a subset of the form $\{\{a,b,c\},\{c,d,e\},\{a,b,e\},\{a,d,e\}\}$, where $I = \{a,\dots,e\}$ 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 $\sum_{i=1}^5 \phi_i \leq \pi$.

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

Applying the above reasoning to the pair $\{\{e,a,b\},\{a,b,c\}\}$ of supports, we get the alternative $\phi_1 + \phi_2 + \phi_5 + \pi - \phi_3 - \phi_4 \geq 2\pi$ or $\phi_1 + \phi_2 + \phi_5 \leq \pi - \phi_3 - \phi_4$. Applying it to the pair $\{\{c,d,e\},\{d,e,a\}\}$, we get $\phi_3 + \phi_4 + \phi_5 + \pi - \phi_1 - \phi_2 \geq 2\pi$ or $\phi_3 + \phi_4 + \phi_5 \leq \pi - \phi_1 - \phi_2$. 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. We demonstrate the argument by an example.

Example: Case 44. Let $A_{ij} = -\cos\phi_{ij}$. Applying Lemma 3.6 to the minimal zero supports $\{1,3,5\}$, $\{2,5,6\}$, $\{1,2,3\}$, $\{2,3,6\}$, we obtain the relation $\phi_{13} + \phi_{15} + \phi_{56} + \phi_{26} + \phi_{23} \leq \pi$. Applying the lemma to the supports $\{1,3,5\}$, $\{2,4,5\}$, $\{1,2,3\}$, $\{1,2,4\}$, we obtain $\phi_{13} + \phi_{35} + \phi_{45} + \phi_{24} + \phi_{12} \leq \pi$. Adding these inequalities and using the relations $\phi_{12} + \phi_{13} + \phi_{23} = \pi$, $\phi_{13} + \phi_{15} + \phi_{35} = \pi$, $\phi_{25} + \phi_{26} + \phi_{56} = \pi$, $\phi_{24} + \phi_{25} + \phi_{45} = \pi$, we obtain the inequality $4\pi - 2\phi_{25} \leq 2\pi$, which leads to a contradiction with the assumption $\phi_{25} \in (0,\pi)$.

In this subsection we established that the manifold of candidate exceptional extremal matrices A with diagonal **1** 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. The subsets differ by how the uncovered elements b_i depend on the angles, and possibly by the constraints on the angles. In Subsection 3.5 below we obtain further constraints on the angles ϕ_i. However, first we shall show in the next subsection how to reduce the number of subsets that have to be considered.

3.4 Symmetry

In some cases the support set $\mathcal{I}$ remains invariant under a non-trivial subgroup of permutations of the indices $1,\dots,6$. This group action can be used to reduce the number of different sub-cases to consider. We shall demonstrate the argument by an example.

Example: Case 2. In this case the matrix A has the form

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

with the angles satisfying the inequalities $\phi_i \in (0,\pi)$, $\phi_1+\phi_2<\pi$, $\phi_1+\phi_3<\pi$. The first order conditions yield the relations $b_1 \geq \cos\phi_2$, $b_1 \geq \cos\phi_3$, $b_2 \geq \cos\phi_1$, the other first order inequalities being consequences of these three. The polyhedron $\mathcal{B}$ defined in Lemma 3.5 is then isomorphic to $\mathbb{R}_+^2$, its unique extreme point corresponding to the values $(b_1,b_2)=(\cos\phi_2,\cos\phi_1)$ in case $\phi_2 \leq \phi_3$ and $(b_1,b_2)=(\cos\phi_3,\cos\phi_1)$ in case $\phi_3 \leq \phi_2$. Thus there exist two sub-cases.

However, the support set $\mathcal{I}$ possesses a symmetry. Namely, the exchange of the indices 3 and 4 leaves $\mathcal{I}$ invariant, but exchanges the angles ϕ_2,ϕ_3 and hence the two sub-cases. As a consequence, we need only to consider the first sub-case, because by possibly applying the symmetry we may always enforce the inequality $\phi_2 \leq \phi_3$. The second sub-case then automatically appears among the images of the obtained exceptional extremal matrices under permutations of the indices.

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

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

In case 9 the symmetry group is trivial, while the number of sub-cases is two. These sub-cases are hence non-isomorphic and need to be considered both.

In case 13 the symmetry group is non-trivial, but reduces the number of sub-cases to only two, which are hence non-isomorphic. The manifolds corresponding to these sub-cases intersect in a submanifold of lower dimension.

In Table 5 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 which can be enforced by the symmetry.

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 be adapted to check, for a given copositive matrix, the presence or absence of minimal zeros with a given support. 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 supports.

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 $\operatorname{supp} v \subset I \subset \operatorname{supp}_{\geq 0}(Av)$.*

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 $\operatorname{supp} v \subset I \subset \operatorname{supp}_{\geq 0}(Av)$.*

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 $\operatorname{supp}\tilde{v} \subset \{1,\dots,|I|\} \subset \operatorname{supp}_{\geq 0}(A_I\tilde{v})$. (The second inclusion must then be an equality.) Padding $\tilde{v}$ with $n-|I|$ zeros at appropriate places, we obtain $v \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$ with $\operatorname{supp} v \subset I \subset \operatorname{supp}_{\geq 0}(Av)$. 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 to either find a vector $v \in \mathbb{R}^6 \setminus (-\mathbb{R}_+^6)$ such that I contains the support of v and is contained in the nonnegative support of Av, or 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 $I \subset \{1,\dots,6\} = \operatorname{supp}_{\geq 0}(Au)$. The equality is ensured by the conditions $(Au)_j \geq 0$ considered in Subsection 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 set individually. These vectors are listed in Table 6 and may depend on the angles ϕ_i.

Index sets of cardinality 5 or 6 always turn 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 by virtue of Lemma 3.9 further reduce the set of ϕ_i in a way such that the non-linear constraints on the ϕ_i mentioned in Subsection 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 have to certify the absence of minimal zeros with additional supports. 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 I. Let $u \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ be such that* supp $u \subset I \subset \mathrm{supp}_{\geq 0}(Au)$*. Set $B = A_I$ and $v = u_I$. Then v is a positive multiple of w_I, and $Bv = 0$.*

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

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 $v^T Bw = 0$. But $Bv \geq 0$ and $w > 0$, which implies $Bv = 0$ and proves our second claim. It follows 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 I having cardinality not equal to 3. In the previous section we obtained a vector $u \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ such that supp $u \subset I \subset \mathrm{supp}_{\geq 0}(Au)$. Set $B = A_I$ and $v = u_I$. If either v has a non-positive element, or $Bv \neq 0$, then by Lemma 3.10 this certifies the absence of a minimal zero with support I. In this way the absence of additional minimal zeros with supports I of cardinality 4 or more is certified for all cases under consideration.

For supports $I = \{i, j, k\}$ 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 as defined in the formulation of 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. Let us demonstrate the argument by examples.

Example: Case 16. The form of the matrix is given in Section 5 below, with $A_{45} = b_1$. The first-order conditions yield the constraints $\phi_1 + \phi_2 + \phi_3 + \phi_5 + \phi_6 \leq \pi$, $\phi_1 + \phi_2 + \phi_4 + \phi_5 + \phi_7 \leq \pi$ on the angles $\phi_j \in (0, \pi)$. The symmetry $(123456) \mapsto (361452)$ allows to enforce also the inequality $\phi_4 + \phi_6 \geq \phi_3 + \phi_7$. The polyhedron $\mathcal{B}$ defined in Lemma 3.5 is isomorphic to $\mathbb{R}_+$, and its extreme point corresponds to the value $b_1 = \max(\cos(\phi_3 - \phi_4), \cos(\phi_6 - \phi_7), \frac{\sin\phi_6 \cos\phi_4 + \sin\phi_3 \cos\phi_7}{\sin(\phi_3 + \phi_6)})$. A priori we have thus three sub-cases to consider.

Consider the index set $I = \{1, 4, 6\}$. Summing the angles corresponding to the off-diagonal entries of the submatrix A_I, we obtain the expression $\pi - \phi_2 - \phi_3 + \pi - \phi_1 - \phi_5 + \phi_6 \geq \pi + 2\phi_6 > \pi$. This certifies copositivity of the submatrix A_I and the absence of a minimal zero with support I. Similar results are obtained for the other index sets of cardinality three, except $I = \{2, 5, 6\}$.

For this I the sum of the angles equals $\phi_4 + \pi - \phi_3 - \phi_6 + \phi_7$. In order for the submatrix A_I to be copositive, we have to demand that this sum be not smaller than π, or equivalently $\phi_4 + \phi_7 \geq \phi_3 + \phi_6$. From this inequality together with $\phi_4 + \phi_6 \geq \phi_3 + \phi_7$ it follows that $\phi_4 \geq \phi_3$. This in turn entails $\phi_4 - \phi_3 \geq |\phi_6 - \phi_7|$, and the maximum in the value of b_1 is achieved by $\cos(\phi_6 - \phi_7)$. In order to guarantee the absence of a zero with support I, we have to assume even the strict inequality $\phi_4 + \phi_7 > \phi_3 + \phi_6$.

Example: Case 23. The form of the matrix A has been given in Subsection 3.1. The first-order conditions yield the relations $\phi_3 + \phi_4 \leq \phi_2$, $\phi_1 + \phi_2 + \phi_5 + \phi_6 \leq \pi$ on the angles $\phi_j \in (0, \pi)$, $j = 1, \dots, 6$.

The polyhedron $\mathcal{B}$ defined in Lemma 3.5 is isomorphic to $\mathbb{R}^3_+$, and its unique extreme point corresponds to the values $b_1 = \cos\phi_4$, $b_2 = \cos\phi_6$, the value of b_3 being given by

$$\max\left(\frac{\sin\phi_5\cos\phi_4 - \sin\phi_6\cos(\phi_1 + \phi_3)}{\sin(\phi_5 + \phi_6)}, \frac{\sin\phi_3\cos\phi_6 - \sin\phi_4\cos(\phi_1 + \phi_5)}{\sin(\phi_3 + \phi_4)}\right).$$

We have therefore to distinguish two sub-cases, depending on which expression realizes the maximum.

Consider the index set $I = \{2, 5, 6\}$. Copositivity of the submatrix A_I implies that $b_3 \geq \cos(\phi_4 + \phi_6)$. Inserting the two possible values for b_3 into this inequality leads in both cases to the equivalent relation $\phi_1 + \phi_3 + \phi_4 + \phi_5 + \phi_6 \geq \pi$. However, from the constraints on the angles it follows that this inequality can only be satisfied as an equality. But then $b_3 = \cos(\phi_4 + \phi_6)$, leading to an additional minimal zero with support I. This excludes the possibility of extremal copositive matrices having this minimal zero support set.

In case 20 this possibility is excluded by the appearance of additional minimal zeros with support of cardinality two, see also [21],[19].

The appearing additional supports for the cases 20–29 are listed in Table 7.

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 subsections we obtained a manifold of exceptional 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 Subsection 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.

In cases 1 – 4 the linear system is simple enough, but in the other 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 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 $u^j \in \mathbb{R}^n$, $j = 1, \dots, m$, are some vectors, and the index pairs (i,j) vary in some subset $\mathcal{J} \subset \{1,\dots,n\} \times \{1,\dots,m\}$. For every $j = 1,\dots,m$, denote by I_j the set of indices i such that $(i,j) \in \mathcal{J}$. As such the system has $\frac{n(n+1)}{2}$ independent variables, namely the entries of B. The following approach allows to reduce both the number of equations and the number of independent variables. We first describe a simplified version, which actually was applied to all of the remaining cases in Table 1 with the exception of 13 and 19.

Let $F \in \mathbb{R}^{n\times r}$ be a matrix, which we choose to make the set $J = \{j \in \{1,\dots,m\} \,|\, F^T u^j = 0\}$ large, although not maximal. Suppose further that there exists a subset $I \subset \{1,\dots,n\}$ 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 $P = (F')^{-1}B_I(F')^{-T} \in \mathcal{S}^r$. Denote $X = FPF^T$ and $D = B - X$. Then the entries of X are linear functions of P, and by construction of P we have $D_I = 0$.

For $j \in J$ we have $Xu^j = 0$ and hence $\sum_{k\in\operatorname{supp} u^j} D_{ik}u^j_k = (Du^j)_i = 0$ for every $i \in I_j$. Therefore, if for $j \in J$, $i \in I_j$ all but one element D_{ik}, $k \in \operatorname{supp} u^j$ vanish, the remaining element must vanish too. Starting from the relations $D_{ik} = 0$, $i,k \in I$, we may hence use certain equations of the linear system on B to show that a number of elements of the difference D vanishes. Any equation $D_{ik} = 0$ obtained this way is equivalent to the relation $B_{ik} = X_{ik}$ and hence expresses the element B_{ik} as a linear function of P.

This allows to use a certain number of equations $(Bu^j)_i = 0$ to express some of the independent variables B_{ik} as functions of a smaller number of variables, namely the elements of P, and hence to reduce the size of the system. We may apply this procedure several times, for instance by defining a second matrix $G \in \mathbb{R}^{n\times s}$, a second index set I' of size s such that the corresponding submatrix G' of G is invertible, and replace the $\frac{s(s+1)}{2}$ variables in the submatrix $B_{I'}$ by the entries of $Q = (G')^{-1}B_{I'}(G')^{-T} \in \mathcal{S}^s$. Then further entries of B may be equal to the corresponding entries of $Y = GQG^T$, and hence can be expressed as linear functions of Q. Some elements B_{ik} may equal both X_{ik} and Y_{ik}. In this case we have to add the corresponding equations $X_{ik} = Y_{ik}$, which are actually relations between the entries of P and Q, to the system.

Let us illustrate the argument by an example.

Example: Case 5. The matrix A is listed below in Section 5 and depends on five angles $\phi_j \in (0,\pi)$. We shall consider the linear system determining extremality in the non-degenerate case $\phi_3 < \phi_4$, $\phi_1+\phi_2+\phi_4+\phi_5 < \pi$. We have 21 equations on the 21 elements of B, namely

$$(Bu^1)_{\{1,2,3,5\}} = (Bu^2)_{\{1,2,3,5,6\}} = (Bu^3)_{\{1,4,5\}} = (Bu^4)_{\{2,4,6\}} = (Bu^5)_{\{3,4,6\}} = (Bu^6)_{\{4,5,6\}} = 0.$$

Let us choose $J = \{3,4,5,6\}$ and $F \in \mathbb{R}^{6\times 2}$ such that the columns of F span the orthogonal complement of the span of u^j, $j \in J$. Let further $I = \{4,5\}$, let $P \in \mathcal{S}^2$ be a matrix-valued variable, set $X = FPF^T$, $D = B - X$, and link P to the elements of B by letting $D_I = 0$. Then $Xu^j = 0$ for all $j \in J$. The equation $(Bu^6)_4 = 0$ then implies $(Du^6)_4 = 0$, which reads $D_{44}u^6_4 + D_{45}u^6_5 + D_{46}u^6_6 = D_{46}u^6_6 = 0$. Hence $(Bu^6)_4 = 0$ can equivalently be rewritten as $D_{46} = 0$. Likewise, $(Bu^6)_5 = 0$ can be rewritten as $D_{56} = 0$. But then the vanishing of $(Bu^6)_6$ is equivalent to the vanishing of D_{66}, and further the vanishing of $(Bu^5)_6, (Bu^5)_4, (Bu^5)_3, (Bu^4)_6, (Bu^4)_4, (Bu^4)_2, (Bu^3)_5, (Bu^3)_4, (Bu^3)_1$ is equivalent to the vanishing of $D_{36}, D_{34}, D_{33}, D_{26}, D_{24}, D_{22}, D_{15}, D_{14}, D_{11}$, respectively. The three equations $(Bu^1)_5 = (Bu^2)_{\{5,6\}} = 0$ determine B_{25}, B_{35}, B_{16} as being equal to $-B_{15}, -B_{15}, -B_{36}$, respectively. As a result, using 15 equations we expressed 18 elements of B as explicit functions of the three elements of P.

Let us now define a non-zero vector $G \in \mathbb{R}^{6\times 1}$ such that $G^T u^j = 0$ for $j = 1,2$, set $I' = \{1\}$, let $Q \in \mathbb{R}$, $Y = GQG^T$, $D' = B - Y$, and link Q to B by letting $D'_{I'} = D_{11} = 0$. Vanishing of $(Bu^1)_1, (Bu^1)^2, (Bu^2)_1, (Bu^2)_3, (Bu^2)_2, (Bu^1)_3$ is then equivalent to the vanishing of D'_{12}, D'_{22}, D'_{13}, D'_{33}, D'_{23}, D'_{23}, respectively. Hence using the remaining 6 equations expresses 6 elements of B as explicit functions of Q.

As a result, the matrix B is completely determined by the four elements of P, Q. However, these four variables cannot be chosen freely, because the sets of elements of B determined by P and Q, respectively, have a non-empty intersection. Equating the two expressions for B_{11}, B_{22}, B_{33}, respectively, we obtain three equations on the four variables. We need to determine only the first three rows and columns of F and G, because the other elements do not participate in the equations linking P to Q. A possible choice is

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

Now the system is small enough to establish by direct calculation that the three equations are linearly independent. Hence the solution space of the system is 1-dimensional, and the matrices A are extremal.

The equations $(Bu^1)_5 = (Bu^2)_{\{5,6\}} = 0$ in the above example did not lead to the vanishing of further elements of the difference matrix D. We may, however, modify the procedure to incorporate this kind of situation. Above we chose F and G such that the rows of these matrices are in a bijection with the index set $\{1,\dots,n\}$. This is not necessary, however. We can chose the number N of rows $f_1,\dots,f_N$ of F arbitrarily and define injections π^j from $\operatorname{supp} u^j$ to the index set $\{1,\dots,N\}$ for a number of minimal zeros u^j, in a way that $\sum_{k\in\operatorname{supp} u^j} f_{\pi^j(k)}u_k^j = 0$.

In the example above, we may append F with a row $f_7 = -f_3$ and define π^2 by $1 \mapsto 7$, $3 \mapsto 3$. Then the vanishing of $(Bu^2)_6$ will entail the vanishing of D_{67}. Another two additional rows allow to incorporate the relations on $(Bu^1)_5, (Bu^2)_5$. We may also truncate G to a vector in $\mathbb{R}^3$.

This augmented procedure will be used in Subsection 4.5 further below.

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 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 Case 19

In this section we consider case 19 of Table 1 with minimal zero support set containing a support of cardinality 4. This case requires a separate consideration.

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 diagonal $\mathbf{1}$, 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 $v = (\sin\phi_{23}, \sin(\phi_{12}+\phi_{23}), \sin\phi_{12}, 0)^T$, and let further $\delta = A_{13} - \cos(\phi_{12}+\phi_{23})$. Then $\delta > 0$, because $A_{\{1,2,3\}} \succ 0$. We also have $Av = (\delta\sin\phi_{12}, 0, \delta\sin\phi_{23}, \star)^T$.

We have $u^TAv = 0$ 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 $u \in \mathbb{R}_{++}^4$. 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

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

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 $u \in \mathbb{R}^4_{++}$. 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

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

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

Lemma 4.4. *Let $A \in \mathcal{COP}^4$ have diagonal $\mathbf{1}$ 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 Subsection 3.1 we may use the minimal zero supports of cardinality 3 to express entries of a copositive matrix A with diagonal $\mathbf{1}$ 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 that A equals

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

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 $u^1, \dots, u^6$ can be represented as the columns of the matrix

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

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

4.3 First order conditions

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

The conditions $(Au^5)_4 \geq 0$, $(Au^5)_2 \geq 0$ 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 $(Au^j)_i > 0$ for all other pairs (i,j) with $i \neq \mathrm{supp}\, u^j$.

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 the non-strict inequalities $(Au^5)_{\{2,4\}}, (Au^2)_6, (Au^3)_6 \geq 0$, the strict inequalities $(Au^1)_{\{1,2,6\}}, (Au^2)_{\{2,3\}}, (Au^3)_{\{3,4\}}, (Au^4)_{\{4,5,6\}}, (Au^5)_3, (Au^6)_{\{1,5\}} > 0$, and the inequality $\phi_1+\dots+\phi_5 < \pi$ hold.

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

The presence of a minimal zero with support $\{2,3,4,6\}$ implies that the submatrix $A_{\{2,3,4,6\}}$ is PSD of rank 3 with a positive kernel vector [17, Corollary 3.8]. In particular, all its proper principal submatrices are positive definite. Note 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

$$A_{\{1,3,4,5,6\}} = FF^T + \begin{pmatrix} 0 & \delta_{13} & 0 & 0 & 0 \\ \delta_{13} & 0 & 0 & 0 & \delta_{36} \\ 0 & 0 & 0 & 0 & \delta_{46} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \delta_{36} & \delta_{46} & 0 & 0 \end{pmatrix},$$

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

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. The Schur complement of its lower right corner has to be positive, which implies

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

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

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

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 get $(Au^4)_6 > 0$.

Further we have

$$\begin{aligned}(Au^4)_4 &= (\cos(\phi_2+\phi_3)+\cos(\phi_1+\phi_4+\phi_5))\sin\phi_5 + \sin(\phi_4+\phi_5)(A_{24}-\cos(\phi_1+\phi_5)) > 0, \\ (Au^2)_2 &= \sin\phi_3(A_{24}-\cos(\phi_1+\phi_5)+\cos(\phi_2+\phi_3+\phi_4)+\cos(\phi_1+\phi_5)) > 0,\end{aligned}$$

because $A_{24} > \cos(\phi_1+\phi_5)$ and $\sum_{i=1}^5 \phi_i \leq \pi$. Likewise $(Au^1)_2, (Au^3)_4 > 0$ by symmetry.

Define

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

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 that 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 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 the inequalities
$(Au^1)_1, (Au^2)_3, (Au^3)_3, (Au^4)_5 > 0$ follow.

This completes the proof. □

4.4 Copositivity

Let us 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 minimal zeros other 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) and the positivity of δ_{14}, δ_{16} 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 superset 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 irreducible 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 with 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 diagonal $\mathbf{1}$ and let its minimal zero support set be given by the support 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 diagonal $\mathbf{1}$ 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 remains 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 $(Bu^j)_i = 0$ coming from the zeros $u^1, \dots, u^5$ determine the elements of B. We shall use the augmented method presented in Subsection 3.6. Set

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

and $\pi^1 : (345) \mapsto (123)$, $\pi^2 : (451) \mapsto (234)$, $\pi^3 : (512) \mapsto (345)$, $\pi^4 : (123) \mapsto (456)$, $\pi^5 : (516) \mapsto (347)$, $I = \{1,2\}$. Relate the elements of B to the elements of $P \in \mathcal{S}^2$ by setting $B_{\{3,4\}} = X_I$, where $X = FPF^T$. Using successively the 17 equations $(Bu^j)_i = 0$, $j = 1,\dots,5$, we obtain

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

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} as both X_{11} and X_{66}. This constraint 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 $(Bu^6)_{\mathrm{supp}\, u^6} = 0$ 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

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

which is obtained from plugging the solution B given by P^1 into (6). 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, which is obtained by plugging the solution B corresponding to P^2 into (6). In this case A is not extremal.

Case $\phi_3+\phi_4+\phi_6 = \phi_7$: Then we have the additional equations $(Bu^5)_2 = (Bu^3)_6 = 0$. These are equivalent to the relation $X_{57} = B_{26}$.

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

$$B_{22}u_{62}^2 + 2B_{26}u_{62}u_{66} + B_{66}u_{66}^2 = B_{33}u_{63}^2 + 2B_{34}u_{63}u_{64} + B_{44}u_{64}^2 \tag{9}$$

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 equation is generated by P^1 from (5) by plugging the corresponding B into (9) and ensures the existence of the solution $B = A$. A second linearly independent solution exists if and only if in addition the relations (8) and

$$\begin{aligned} &\cos(\phi_1+\phi_2+\phi_3+\phi_4-\phi_5)u_{62}^2 - 2\cos(\phi_1+\phi_2-\phi_5-\phi_6)u_{62}u_{66} + \\ &+ \quad \cos(\phi_1+\phi_2-\phi_3-\phi_4-\phi_5-2\phi_6)u_{66}^2 = \cos(\phi_1+\phi_2+\phi_3+\phi_4+\phi_5)u_{63}^2 - \\ &- \quad 2\cos(\phi_2+\phi_3+\phi_4+\phi_5)u_{63}u_{64} + \cos(\phi_1-\phi_2-\phi_3-\phi_4-\phi_5)u_{64}^2 \end{aligned} \tag{10}$$

are satisfied, where (10) is generated by P^2 from (5) by plugging the corresponding B into (9). 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 diagonal $\mathbf{1}$ are given by*

(i) all matrices (1) *with $\phi_i \in (0,\pi)$, $\phi_1+\dots+\phi_5 < \pi$, $\phi_9 = \pi+\phi_2-\phi_6$, $\phi_3+\phi_4+\phi_6 < \phi_7$, $A_{\{2,3,4\}} \succ 0$, $A_{\{2,3,4,6\}}u = 0$ 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 $\phi_i \in (0,\pi)$, $\phi_1+\dots+\phi_5 < \pi$, $\phi_9 = \pi+\phi_2-\phi_6$, $\phi_3+\phi_4+\phi_6 = \phi_7$, $A_{\{2,3,4\}} \succ 0$, $A_{\{2,3,4,6\}}u = 0$ for some $u = (u_{62},u_{63},u_{64},u_{66})^T \in \mathbb{R}^4_{++}$, except those satisfying simultaneously* (8) *and* (10)*;*

(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 $\phi_1,\dots,\phi_6$ and the 4 non-zero elements of u^6, constrained by (7) and a normalizing constraint, e.g., $||u^6|| = 1$. The matrices in (ii) 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

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

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

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

Bypassing the system of equations on A involving the zero u^6, the element A_{24} can be determined from the other elements by setting the determinant of $A_{\{2,3,4,6\}}$ to zero.

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 diagonal entries in $\{0,1\}$ which may depend 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 case 19 the matrix A depends also on the minimal zero u^6 with support of cardinality 4.

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 $(Au^j)_i \geq 0$ 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

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

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

Case 8

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

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

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

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

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 u, 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 (10). In generic position a point in angle space determines a 1-dimensional curve of matrices corresponding to different kernel vectors u. The equation linking a_{24}, a_{36} can be obtained by setting $\det A_{\{2,3,4,6\}}$ to zero.

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, 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 $C = DPAP^TD$.*

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 $(Au^j)_i \geq 0$ 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, non-isomorphic (with respect to permutation of the indices) strata of the same dimension corresponding to the same support set.

In Table 8 we present the dimensions of the mutually non-isomorphic strata of exceptional extremal matrices with diagonal **1** 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. At lower order, if the minimal zero support set does not cover an off-diagonal element, this element is nevertheless determined by virtue of Lemma 3.2. However, at order 6 we may obtain elements b_i in the parameterized matrix which cannot a priori be assigned a value depending on the entries of the minimal zeros. 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 the strategy is different from [16], where first the irreducible matrices are classified and then checked for extremality a posteriori.

We obtained 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 Subsection 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. It can be shown that this is not the only 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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Table 1: Candidate minimal support sets $\mathcal{I}$ of exceptional extreme matrices in $\mathcal{COP}^6$

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 matrices with this minimal zero support set exist
2	3	{1,2},{1,3},{1,4},{2,5},{3,5,6},{4,5,6}	
3	4	{1,2},{1,3},{1,4},{2,5,6},{3,5,6},{4,5,6}	
4	5	{1,2},{1,3},{2,4},{3,4,5},{1,5,6},{4,5,6}	
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 extremality enforce additional minimal zero supports
21	11	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6}	
22	12	{1,2},{2,3,4},{3,4,5},{4,5,6},{2,5,6},{2,3,6}	
23	17	{1,2},{1,3,4},{2,3,5},{3,4,5},{2,4,6},{3,4,6}	
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 minimal zeros is a proper subspace
31	10	{1,2},{1,3,4},{1,3,5},{2,3,6},{3,4,6},{3,5,6}	
32	14	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{3,5,6}	
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 are incompatible
44	29	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{2,3,6},{2,5,6}	

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

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 3: Supports of linearly dependent minimal zeros. The minimal zero with barred support is removed.

Case No.	supports	Case No.	supports
30	~~$\{2,4,5\}$~~, $\{3,4,5\}$, $\{2,4,6\}$, $\{3,4,6\}$	39	~~$\{1,2,3\}$~~, $\{1,2,4\}$, $\{1,3,6\}$, $\{1,4,6\}$
31,32	~~$\{1,3,4\}$~~, $\{1,3,5\}$, $\{3,4,6\}$, $\{3,5,6\}$		~~$\{1,3,6\}$~~, $\{1,4,6\}$, $\{3,5,6\}$, $\{4,5,6\}$
33,34,35	~~$\{1,2,3\}$~~, $\{1,2,4\}$, $\{1,3,6\}$, $\{1,4,6\}$	40	~~$\{1,2,3\}$~~, $\{1,2,4\}$, $\{1,3,5\}$, $\{1,4,5\}$
36,37	~~$\{1,2,3\}$~~, $\{1,2,4\}$, $\{1,3,5\}$, $\{1,4,5\}$		~~$\{1,2,4\}$~~, $\{1,4,5\}$, $\{2,4,6\}$, $\{4,5,6\}$
38	~~$\{1,3,4\}$~~, $\{1,3,5\}$, $\{3,4,6\}$, $\{3,5,6\}$		~~$\{1,3,5\}$~~, $\{1,4,5\}$, $\{3,5,6\}$, $\{4,5,6\}$
	~~$\{2,4,6\}$~~, $\{3,4,6\}$, $\{2,5,6\}$, $\{3,5,6\}$		

Table 4: Equalities $(Au^j)_k = 0$ determining the variables b_i

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 5: Symmetry groups, their generators, and enforced inequalities

Case No.	Generator(s)	Group	Inequalities
1	$(1,3,2,4,6,5)$	S_2	
2	$(1,2,4,3,5,6)$	S_2	$\phi_2 \le \phi_3$
3	$(1,3,2,4,5,6); (1,2,4,3,5,6);$ $(1,2,3,4,6,5)$	$S_3 \times S_2$	$\phi_4 \le \phi_3 \le \phi_2$
5	$(1,3,2,4,5,6)$	S_2	$\phi_3 \le \phi_4$
6	$(1,3,2,5,4,6)$	S_2	$\phi_2 + \phi_4 + \phi_5 \le \pi$
7	$(6,5,4,3,2,1)$	S_2	$\phi_1 \le \phi_5$
8	$(2,1,6,4,5,3)$	S_2	$\phi_3 + \phi_4 \le \phi_1 + \phi_6$
11	$(2,1,4,3,5,6)$	S_2	
13	$(6,5,4,3,2,1); (6,1,2,3,4,5)$	D_6	$\phi_1 + \phi_2 + \phi_3 \ge \phi_4 + \phi_5 + \phi_6$, $\phi_3 + \phi_4 + \phi_5 \ge \phi_1 + \phi_2 + \phi_6$
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	$\phi_4 + \phi_6 \ge \phi_3 + \phi_7$
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	$\phi_7 - \phi_3 - \phi_4 - \phi_6 \ge \phi_6 + \phi_9 - \pi - \phi_2$

Table 6: Copositivity certifying vectors for index subsets of cardinality 4

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	$\{1,2,4,5\},\{1,3,4,6\}$	$e_4 \cos\phi_4 + e_5$, $e_1 + e_6$
	$\{2,3,5,6\}$	$e_2 + \cos\phi_2 e_3$
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 7: Additionally appearing minimal zero support

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 8: Dimensions of strata of extremal matrices with diagonal **1**

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		