

# Problem 1: extreme rays of the copositive cone $\mathcal{C}^n$

## Motivation

Copositive matrices appear to have been introduced in 1952 by Motzkin [45]. A real symmetric  $n \times n$  matrix  $A$  is called *copositive* if  $x^T A x \geq 0$  for all  $x \in \mathbb{R}_+^n$ . The set of copositive matrices forms a convex cone, the *copositive cone*  $\mathcal{C}^n$ .

The matrix cone  $\mathcal{C}^n$  is of interest for optimization, as various difficult non-convex optimization problems can be reformulated as conic programs over the copositive cone, so-called *copositive programs*. Among these are combinatorial problems such as the bandwidth problem [49], graph partitioning [50], computing the stability number [21], clique number [57], and chromatic number [32] of graphs, and the quadratic assignment problem [51]. Copositive formulations have been derived for quadratic programming problems [52, 12, 9] and mixed-integer programs [20]. The connection of the copositive cone with sufficient optimality conditions for quadratic programming, i.e., the problem of minimizing a quadratic function under linear constraints, has been recognized already in the 70s [40, Theorem 3.2.3]. For quadratically constrained quadratic programming problems with additional linear constraints copositive relaxations are tighter than standard Lagrangian semi-definite relaxations [11]. In [44, 42, 19, 8] copositive matrices are used for determining Lyapunov functions for switched linear dynamical systems with state confined to the positive orthant or, more generally, to a polyhedral cone. More applications of copositive programming can be found in the surveys [30, 10].

Verifying copositivity of a given matrix is a co-NP-complete problem [46]. Likewise, verifying whether a given linear hyperplane in the space  $\mathcal{S}^n$  of  $n \times n$  real symmetric matrices is supporting to  $\mathcal{C}^n$  at the zero matrix is NP-hard [28]. This is not surprising given the extraordinary descriptive power of copositive programs. Therefore much research has been focussed on finding tractable approximations of the copositive cone, in particular, semi-definite approximations.

The commonest approximation of the cone  $\mathcal{C}^n$  is that by the sum of the cone  $\mathcal{S}_+^n$  of positive semi-definite matrices and the cone  $\mathcal{N}^n$  of element-wise nonnegative symmetric matrices. In [40] the matrices in this sum are called *stochastically copositive*. It is a classical result by Diananda [22, Theorem 2] that for  $n \leq 4$  the relation  $\mathcal{C}^n = \mathcal{S}_+^n + \mathcal{N}^n$  holds, i.e., copositivity and stochastic copositivity are equivalent. In general, stochastic copositivity merely implies copositivity, and  $\mathcal{S}_+^n + \mathcal{N}^n \subset \mathcal{C}^n$ . A. Horn showed that for  $n \geq 5$  this inclusion is indeed strict [22, p.25]. Matrices which are copositive but not stochastically copositive are called *exceptional*, a term that has been coined in [41].

With the appearance of semi-definite programming more sophisticated approximations of  $\mathcal{C}^n$  have been elaborated in order to solve copositive programs. In [47] a hierarchy of inner semi-definite approximations for  $\mathcal{C}^n$  has been constructed, with the sum  $\mathcal{S}_+^n + \mathcal{N}^n$  being its simplest member. It is based on representing the copositive cone as a cone of positive polynomials and applying sum of squares approximations. In [9] this hierarchy has been relaxed to a hierarchy of polyhedral inner approximations. In [43] a hierarchy of outer semi-definite approximations of  $\mathcal{C}^n$  has been proposed based on moments involving the exponential measure on  $\mathbb{R}_+^n$ . All these hierarchies are asymptotically exact, i.e., the approximating cones tend to  $\mathcal{C}^n$  as the order of the approximation tends to infinity. The complexity of the approximating cones grows exponentially with the order, however.

There exist also methods which deal directly with the data of the copositive program under consideration. In [18, 19, 57] branch-and-bound methods based on a tree of polyhedral approximations of the copositive cone have been proposed to check membership in this cone and to solve copositive programs. In [14] a local descent method was proposed which works with the conic dual to the copositive program. In [13, 31] copositivity is checked by a decomposition of a non-convex function as a difference of two convex functions.

For further surveys on copositive matrices see [38, 15], for a list of open problems see [6]. Closely related to the copositive cone  $\mathcal{C}^n$  is its dual  $\mathcal{C}_n^*$ , the *completely positive cone*. For surveys on completely positive matrices see, e.g., [7, 15, 25].

## Extreme copositive matrices

We focus on a particular topic, namely the extreme rays of  $\mathcal{C}^n$ . An element  $x \in K$  is called an *extremal* element of a regular convex cone  $K$  if a decomposition  $x = x_1 + x_2$  of  $x$  into elements  $x_1, x_2 \in K$  is only possible if  $x_1 = \lambda x$ ,  $x_2 = (1 - \lambda)x$  for some  $\lambda \in [0, 1]$ . The set of positive multiples of an extremal element is called an *extreme ray* of  $K$ . 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 difficult cone 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. Since the extreme rays of a cone determine the facets of its dual cone, they are also important tools for the study of this dual cone [23, 56, 16, 17, 55, 54].

It is therefore not surprising that the extreme rays of  $\mathcal{C}^n$  have been the subject already of many of the first papers on copositive matrices. The extreme rays of  $\mathcal{C}^n$  which are elements of the sum  $\mathcal{S}_+^n + \mathcal{N}^n$  have been completely classified in [33]. Since  $\mathcal{C}^n = \mathcal{S}_+^n + \mathcal{N}^n$  for  $n \leq 4$ , this yields also a complete classification of the extreme rays of  $\mathcal{C}^n$  for  $n \leq 4$ . The first exceptional extreme copositive form has been found by A. Horn, according to [22, p.25]. This *Horn form* is a circulant  $5 \times 5$  matrix with entries in  $\{-1, +1\}$ . In [3, Theorem 3.8] Baumert gave a procedure to construct an extreme ray of  $\mathcal{C}^{n+1}$  from an extreme ray of  $\mathcal{C}^n$ , by duplicating a row and the corresponding column of the original matrix. Starting with the Horn form, he was then able to construct explicit exceptional extreme copositive matrices of every size  $n \geq 5$ . Extreme copositive matrices which cannot be obtained by this procedure have been called *basic* in [1].

In his thesis [2] and his paper [3] Baumert laid the foundation of a theory of extremal exceptional copositive forms. He recognized the importance of the symmetry group  $\mathcal{G}_n$  of the cone  $\mathcal{C}^n$ , which consists of maps of the form  $A \mapsto PDADP^T$ , where  $D$  is a positive definite diagonal matrix, and  $P \in S_n$  is a permutation matrix. The elements of this symmetry group preserve the sum  $\mathcal{S}_+^n + \mathcal{N}^n$  and hence also the property of a copositive matrix of being exceptional. Baumert showed that an exceptional extreme copositive matrix has positive diagonal elements and hence can be scaled to a matrix with all diagonal elements equal to 1 by the action of  $\mathcal{G}_n$ . By a result from [33] he concluded that the off-diagonal elements of the scaled extremal exceptional matrix have all to be in the interval  $[-1, +1]$ .

The extremal exceptional matrices of  $\mathcal{C}^n$  with elements in  $\{-1, +1\}$  have been classified completely in [4] for  $n \leq 7$ , where it has been shown that they can all be obtained from the Horn form by a group action and the above-mentioned procedure of duplicating rows and columns, a result which does not hold anymore for  $n = 8$  [1]. For general  $n$  the extremal exceptional matrices with elements in  $\{-1, +1\}$  have been characterized independently in [34, 1]. The extreme exceptional matrices in  $\mathcal{C}^n$  with elements from the set  $\{-1, 0, +1\}$  have been characterized in [39].

Since an exceptional copositive matrix cannot be a multiple of an element in the sum  $\mathcal{S}_+^n + \mathcal{N}^n$ , subtraction of a non-zero such element from an extreme exceptional copositive matrix will lead to a matrix which is no more copositive. This fact has early been recognized and led to a number of conditions on exceptional copositive matrices which are weaker than extremality but more tractable. Baumert called a copositive matrix *reduced* if one cannot subtract a non-zero nonnegative matrix from it without leaving the copositive cone [3], a condition which has been initially introduced and put to use in [22]. Baumert refined this condition by requiring the subtracted nonnegative matrix to be proportional to the extremal element  $E_{ij}$  of  $\mathcal{N}^n$ , where  $E_{ij}$  is the symmetric  $n \times n$  matrix having a 1 at positions  $(i, j)$  and  $(j, i)$  and whose other elements all equal zero. He furnished a necessary and sufficient condition on a copositive matrix to be reduced with respect to  $E_{ii}$  [3, Theorem 3.4] and conjectured a similar condition for reducedness with respect to  $E_{ij}$  with  $i \neq j$  [4, Conjecture 4.1], refuted later in [39] by a counterexample of order  $n = 7$ .

These conditions are expressed in terms of the presence or absence of zeros with certain properties. The importance of the concept of zeros of a copositive matrix has been recognized already by Diananda who introduced it in [22]. A nonzero vector  $u \in \mathbb{R}_+^n$  is called a *zero* of a copositive matrix  $A \in \mathcal{C}^n$  if  $u^T A u = 0$ . A zero  $u$  of  $A$  is called *isolated* if in a neighbourhood of  $u$  there are no other zeros of  $A$  other than the multiples of  $u$ . For a vector  $u \in \mathbb{R}^n$  we define its *support* as  $\text{supp } u = \{i \in \{1, \dots, n\} \mid u_i \neq 0\}$ , i.e., as the index set of the non-zero elements of  $u$ . The possible supports of a nonnegative vector are in one-to-one correspondence with the faces of the nonnegative orthant where this vector may be situated. However, a zero  $u$  of a copositive form represents a global minimum of this form on the nonnegative orthant. Therefore the first and second order optimality conditions at  $u$  are determined by its support. The set of supports of the zeros of a copositive matrix is hence an informative combinatorial characteristic of this matrix which has attracted a lot of attention and is an important mathematical tool in the analysis of copositive matrices and the copositive cone. We shall call this set the *support set* of the copositive matrix in question. In [22, 33, 2, 3, 4] many necessary conditions on the support set of an extremal or a reduced exceptional copositive matrix have been found, and on the other hand, many conditions on the matrix have been established which are determined by its support set. Let us remark that instead of the support as defined here, Baumert defined and used the equivalent notion of the *pattern* of a zero. This notion turned out to be less convenient than that of the support, by which it has been superseded nowadays. Properties of zeros and algorithms to find the zero set of copositive matrices have been recently considered in [23] in application to a study of the faces of the copositive cone and its dual.

In [2, 4] Baumert discovered that the cone  $\mathcal{C}^5$  possessed a family of exceptional extreme elements with a

support set which is different from that of the Horn form, and gave an explicit matrix from this family. Key to this finding was the introduction of the concept of *maximal zero*. A maximal zero  $u$  of a copositive matrix  $A$  is a zero such that there does not exist another zero  $v$  of  $A$  such that  $\text{supp } u \subset \text{supp } v$  strictly.

After the paper [39] from the early 70s research on the extreme elements of the copositive cone came to a halt for many years, until the revival which occurred in the current decade.

## Recent results

The facial structure of the copositive cone, including the extreme rays, has been studied in [23].

In [36] a complete description of the extreme rays of the cone  $\mathcal{C}^5$  was given. The strategy of the proof follows the one outlined by Baumert [2], by replacing extremality by the weaker condition of reducedness with respect to nonnegative matrices, which is easier to handle. However, two new ideas have been necessary for a successful implementation.

The first one has been to introduce a trigonometric parametrization of the extreme matrices with all diagonal elements equal to 1. As mentioned above, such matrices have their off-diagonal elements in the interval  $[-1, +1]$ , which can be parameterized by  $\cos \varphi$  with the angle  $\varphi$  running through the interval  $[0, \pi]$ . It turns out that the family of extreme elements discovered by Baumert becomes affine in these angles and its range is delimited by linear inequalities on the angles. As a result, the manifold of these exceptional extreme  $5 \times 5$  matrices, which have initially been called *T*-matrices in [36], can be described in a closed analytic form. The reason for this to happen is the special structure of Cayleys nodal cubic surface which models the zero set of the determinant of real symmetric  $3 \times 3$  matrices with diagonal elements equal to 1. This surface decomposes into a union of four planes when undergoing the above trigonometric transformation. However, the optimality conditions associated with the isolated zeros of the extreme forms of  $\mathcal{C}^5$  in question force the  $3 \times 3$  principal submatrices of the forms corresponding to the supports of the zeros to be singular. This will happen anytime a zero of a copositive form has a support of cardinality less or equal to three. Thus the proposed trigonometric approach will lead to similar results for any family of extreme rays of  $\mathcal{C}^n$  whose zeros have supports with cardinality less or equal to three, independently of the order  $n$ .

The second critical ingredient was to derive a necessary and sufficient condition on a copositive matrix to be reduced with respect to the extreme element  $E_{ij}$  of the nonnegative cone for  $i \neq j$ . Baumert has conjectured such a condition in [4, Conjecture 4.1] and was able to prove that his families of extreme elements of  $\mathcal{C}^5$  were indeed exhaustive, assuming the conjecture. Namely, he provided a partial classification of the support sets of matrices in  $\mathcal{C}^5$  which are reduced with respect to the cone  $\mathcal{N}^5$ , which would have been complete were the conjecture true. This classification was completed in [26], by deriving the correct condition for reducedness with respect to  $E_{ij}$ . It turned out that this led to additional families of reduced matrices, but none of them were extremal.

The study of the cone  $\mathcal{C}^5$  was completed in [27], where it was shown that the second relaxation in Parrilos hierarchy [47] was exact in describing the subset of  $5 \times 5$  copositive matrices with all diagonal elements equal to 1.

The classification of the extreme rays of  $\mathcal{C}^5$  was based on a tedious classification of the possible support sets of copositive  $5 \times 5$  matrices which are reduced with respect to the nonnegative cone  $\mathcal{N}^5$ , initiated by Baumert in [4] and completed in [26]. For the extension to copositive cones of order  $n > 5$  a more systematic study of support sets of exceptional extremal copositive matrices was necessary.

In [37] the concept of minimal zeros was introduced, as opposed to the maximal zeros studied by Baumert in [2]. Here a zero  $u$  of a copositive form  $A$  is called *minimal* if for no other zero  $v$  of  $A$ , the support of  $v$  is a strict subset of the support of  $u$ . In contrast to maximal zeros, or zeros in general, a minimal zero of a copositive matrix is determined up to scaling by a positive constant only by its support and by the matrix itself. Thus a copositive matrix can essentially have only a finite number of minimal zeros, which opens the way to a combinatorial approach. The set of supports of all minimal zeros of a copositive matrix  $A$  is called the *minimal support set* of  $A$ .

Also in [37] an extension of the concept of reducedness was presented. An exceptional extreme copositive matrix  $A \in \mathcal{C}^n$  is not only reduced with respect to the nonnegative cone, but for the same reasons must also be reduced with respect to the positive semi-definite cone, i.e., it cannot be decomposed into a non-trivial sum  $A = C + P$ , where  $C$  is copositive and  $P$  is positive semi-definite. This reducedness requirement leads to additional conditions on the support set of the extremal matrix.

The main result of [37] is a set of necessary conditions on the minimal support set of an exceptional copositive matrix which is reduced with respect to both  $\mathcal{S}_+^n$  and  $\mathcal{N}^n$ . When applied retrospectively to the cone  $\mathcal{C}^5$ , these conditions are strong enough to single out exactly the two support sets which correspond to the two types of

exceptional extreme rays of  $\mathcal{C}^5$ , namely the orbits of the Horn form and the  $T$ -matrices. For  $n = 6$ , the conditions reduce the number of potential minimal support sets to 44, which makes the classification of the extreme rays of  $\mathcal{C}^6$  possible with a manageable effort. Surprisingly, for some applications the list of support sets itself suffices, without explicit knowledge of the extreme rays [54].

As mentioned above, in previous work the condition of extremality was substituted by the weaker condition of reducedness, because the latter is easier to handle. However, it is a trivial observation that extremality itself can also be described by a reducedness condition. Namely, a copositive matrix is extremal if and only if one cannot subtract another copositive matrix from it without leaving the copositive cone, except when this other matrix is a multiple of the original matrix. The reducedness condition with respect to general convex cones was studied in the paper [29].

The concept of reducedness is generalized in the following way. A copositive matrix  $A \in \mathcal{C}^n$  is called *reduced* with respect to another copositive matrix  $C$  if for every  $\delta > 0$ , we have  $A - \delta C \notin \mathcal{C}^n$ , and it is called reduced with respect to a subset  $\mathcal{M} \subset \mathcal{C}^n$  if it is irreducible with respect to all nonzero elements  $C \in \mathcal{M}$ .

The paper [29] has a strong convex analysis flavour. Its main result is a necessary and sufficient condition on a pair  $(A, B)$ , where  $A \in \mathcal{C}^n$  and  $B \in \mathcal{S}^n$ , for the existence of a scalar  $\delta > 0$  such that  $A + \delta B \in \mathcal{C}^n$ . For fixed  $A$ , the set of all such matrices  $B \in \mathcal{S}^n$  forms a convex cone  $\mathcal{K}^A$ , which is referred to as the *cone of feasible directions* [48]. This cone has been expressed in terms of the zeros of  $A$  and their supports.

The obtained description of the cone  $\mathcal{K}^A$  is a powerful tool. It allows to compute the minimal face of  $A$ , see [5, 53] for further information on faces of a convex set or cone. In particular, a simple test of extremality of  $A$  is obtained, which amounts to checking the rank of a certain matrix constructed from the minimal zeros of  $A$ . The necessary and sufficient conditions for the reducedness of  $A$  with respect to a nonnegative matrix  $C \in \mathcal{N}^n$  or a positive semi-definite matrix  $C \in \mathcal{S}_+^n$ , which have been given in [26] and [37], respectively, are generalized to the case of arbitrary matrices  $C \in \mathcal{C}^n$ . The conditions in [26] and [37] follow as particular cases.

In [24] simpler criteria in the form of subsets of vectors for checking copositivity of a given matrix have been described.

## Problem description

Let us now summarize the elaborated approach to exceptional extremal copositive matrices. We divide our study in two steps. First we look at the possible minimal support sets of extremal copositive matrices, constrained by necessary conditions on the zeros. This step can be characterized as a qualitative analysis, because the main object is of a combinatorial nature. Then we consider which extremal copositive matrices exist with a given support set. This step is of a quantitative nature, and essentially boils down to solving underdetermined systems of algebraic equations.

Both steps encounter difficulties when the order of the copositive matrices increases. One problem is the exploding number of possible minimal support sets, and the other is the increasing complexity of the system of equations. There are two regimes where these problems seem manageable. If the supports of the zeros are small, of cardinality 2 or 3, then the trigonometric parametrization of the extremal matrices scaled such that their diagonal elements equal 1 yields a linear system on the parameterizing angles, and the corresponding families of extremal matrices can explicitly be written down. If the supports are large, then the corresponding system of equations is rigid enough to prevent a too complex structure of the extremal matrices.

In the case of the cone  $\mathcal{C}^6$  a complete classification of the extreme rays is still attainable. On the one hand, with 44 the number of minimal support sets to study is moderate. The prospective minimal support sets are listed in Table 1, up to permutations of the index set  $\{1, \dots, 6\}$ . On the other hand, every minimal support set contains only zeros with support of size 2 or 3, which is the case of small supports, or of size  $n - 2 = 4$ , which falls in the category of large supports. The treatment of each of the cases is hence expected to be feasible without the encounter of major difficulties.

The proposed problem consists in determining all exceptional extremal copositive matrices with unit diagonal for each of the listed minimal support sets. The cases can be solved independently of each other, some of them have already been solved. For an up to date list of the solved cases including the solutions see [35].

We now sketch a path to the solution of the problem. For a given minimal support set, each minimal zero imposes conditions on an extremal copositive matrix  $A$  with unit diagonal having this support set. Below we list these conditions [26, 37]:

**Zeros with support of size 2:** If  $\{i, j\}$  is the support of a zero of  $A$ , then  $A_{ij} = -1$ .

No.	$\text{supp } \mathcal{V}_{\min}^A$	No.	$\text{supp } \mathcal{V}_{\min}^A$
1	$\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{3,6\},\{5,6\}$	23	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{2,4,6\},\{3,4,5,6\}$
2	$\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{3,6\},\{4,5,6\}$	24	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{3,4,6\},\{3,5,6\}$
3	$\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{3,5,6\},\{4,5,6\}$	25	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{3,4,6\},\{4,5,6\}$
4	$\{1,2\},\{1,3\},\{1,4\},\{2,5,6\},\{3,5,6\},\{4,5,6\}$	26	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{1,4,5\},\{2,3,6\},\{2,4,6\}$
5	$\{1,2\},\{1,3\},\{2,4\},\{3,4,5\},\{1,5,6\},\{4,5,6\}$	27	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{1,4,5\},\{2,3,6\},\{3,4,6\}$
6	$\{1,2\},\{1,3\},\{1,4,5\},\{2,4,6\},\{3,4,6\},\{4,5,6\}$	28	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{2,4,5\},\{3,4,5\},\{2,3,6\}$
7	$\{1,2\},\{1,3\},\{2,4,5\},\{3,4,5\},\{2,4,6\},\{3,4,6\}$	29	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{2,4,5\},\{2,3,6\},\{2,5,6\}$
8	$\{1,2\},\{1,3\},\{2,4,5\},\{3,4,5\},\{2,4,6\},\{3,5,6\}$	30	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{2,4,5\},\{3,4,6\},\{3,5,6\}$
9	$\{1,2\},\{3,4\},\{1,3,5\},\{2,4,6\},\{1,5,6\},\{4,5,6\}$	31	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{2,4,5\},\{1,5,6\},\{2,5,6\}$
10	$\{1,2\},\{1,3,4\},\{1,3,5\},\{2,3,6\},\{3,4,6\},\{3,5,6\}$	32	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{2,4,5\},\{1,5,6\},\{4,5,6\}$
11	$\{1,2\},\{1,3,4\},\{1,3,5\},\{1,4,6\},\{2,5,6\},\{3,5,6\}$	33	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{2,4,5\},\{3,5,6\},\{4,5,6\}$
12	$\{1,2\},\{1,3,4\},\{1,3,5\},\{1,4,6\},\{3,5,6\},\{4,5,6\}$	34	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{2,4,6\},\{3,5,6\},\{4,5,6\}$
13	$\{1,2\},\{1,3,4\},\{1,3,5\},\{2,4,6\},\{3,4,6\},\{2,5,6\}$	35	$\{1,2,3,4\},\{1,2,3,5\},\{1,2,4,6\},\{1,3,5,6\},\{2,4,5,6\},\{3,4,5,6\}$
14	$\{1,2\},\{1,3,4\},\{1,3,5\},\{2,4,6\},\{3,4,6\},\{3,5,6\}$	36	$\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{4,5\},\{3,6\},\{5,6\}$
15	$\{1,2\},\{1,3,4\},\{1,3,5\},\{2,4,6\},\{3,4,6\},\{4,5,6\}$	37	$\{1,2\},\{1,3,4\},\{1,3,5\},\{1,4,6\},\{2,5,6\},\{3,5,6\},\{4,5,6\}$
16	$\{1,2\},\{1,3,4\},\{1,3,5\},\{2,4,6\},\{3,5,6\},\{4,5,6\}$	38	$\{1,2\},\{1,3,4\},\{1,3,5\},\{2,4,6\},\{3,4,6\},\{2,5,6\},\{3,5,6\}$
17	$\{1,2\},\{1,3,4\},\{2,3,5\},\{3,4,5\},\{2,4,6\},\{3,4,6\}$	39	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{1,4,6\},\{2,5,6\},\{3,5,6\}$
18	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{1,4,6\},\{1,5,6\}$	40	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{1,4,6\},\{3,5,6\},\{4,5,6\}$
19	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{1,4,6\},\{2,5,6\}$	41	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{2,4,6\},\{3,4,6\},\{3,5,6\}$
20	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{1,4,6\},\{3,5,6\}$	42	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{2,4,6\},\{3,5,6\},\{4,5,6\}$
21	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{2,4,6\},\{3,4,6\}$	43	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{1,4,6\},\{2,5,6\},\{3,5,6\},\{4,5,6\}$
22	$\{1,2,3\},\{1,2,4\},\{1,2,5\},\{1,3,6\},\{2,4,6\},\{3,5,6\}$	44	$\{1,2,3\},\{1,2,4\},\{1,3,5\},\{1,4,5\},\{2,3,6\},\{2,4,6\},\{3,5,6\},\{4,5,6\}$

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

**Minimal zeros with support of size 3:** If  $\{i, j, k\}$  is the support of a minimal zero of  $A$ , then the  $3 \times 3$  principal submatrix  $(A_{rs})_{r,s=i,j,k}$  of  $A$  is given by  $\begin{pmatrix} 1 & -\cos \varphi_1 & -\cos \varphi_2 \\ -\cos \varphi_1 & 1 & -\cos \varphi_3 \\ -\cos \varphi_2 & -\cos \varphi_3 & 1 \end{pmatrix}$  with positive angles satisfying  $\varphi_1 + \varphi_2 + \varphi_3 = 0$ .

**Minimal zeros with support of size 4:** If  $\{i, j, k, l\}$  is the support of a minimal zero of  $A$ , then the  $4 \times 4$  principal submatrix  $(A_{rs})_{r,s=i,j,k,l}$  of  $A$  is positive semi-definite of rank 3 and with the 1-dimensional kernel generated by a vector with positive entries.

**First order optimality condition:** Every zero  $u$  of  $A$  is a global minimum of the quadratic function  $f(x) = x^T A x$  over the nonnegative orthant. The first-order optimality condition then reads  $Au \geq 0$ , where the inequality is to be interpreted element-wise.

These conditions help to reduce the number of parameters entering  $A$  from the initial number of 15 independent off-diagonal elements to a few, defining an algebraic variety of the corresponding dimension. For the matrices in this variety one has to check copositivity and extremality. The second task can be reduced to checking feasibility of a linear system of equations. We have the following result [29, Theorem 17].

Let  $A \in \mathcal{C}^n$  be a copositive matrix. Then  $A$  is extremal if and only if the following linear system of equations on the real symmetric  $n \times n$  matrix  $B$  has no solutions which are linearly independent from  $A$ :  $(Bu)_i = 0$  for all minimal zeros  $u$  of  $A$  and for all indices  $i$  not in the support of  $Au$ .

Checking copositivity of a matrix is more subtle. The criteria in [24] can be helpful.

Once all exceptional extreme rays of  $\mathcal{C}^6$  are found, one can proceed to constructing semi-definite descriptions of the unit diagonal section of this cone, in the spirit of [27]. This opens the way to the design of algorithms for solving conic optimization problems over this cone.

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