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# Generating extreme copositive matrices near matrices obtained from COP-irreducible graphs

Maxim Manainen \*    Mikhail Seliugin \*    Roman Tarasov \*    Roland Hildebrand †

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## Abstract

In this paper we construct new families of extremal copositive matrices in arbitrary dimension by an algorithmic procedure. Extremal copositive matrices are organized in relatively open subsets of real-algebraic varieties, and knowing a particular such matrix  $A$  allows in principle to obtain the variety in which  $A$  is embedded by solving the corresponding system of algebraic equations. We show that if  $A$  is a matrix associated to a so-called COP-irreducible graph with stability number equal 3, then by a trigonometric transformation these algebraic equations become linear and can be solved by linear algebra methods. We develop an algorithm to construct and solve the corresponding linear systems and give examples where the variety contains singularities at the initial matrix  $A$ . For the cycle graph  $C_7$  we completely characterize the part of the variety which consists of copositive matrices.

## 1 Introduction

Copositive matrices appear to have been introduced in 1952 by Motzkin [1]. A real symmetric  $n \times n$  matrix  $A$  is called *copositive* if  $x^T Ax \geq 0$  for all  $x \in \mathbb{R}_+^n$ . The set of copositive matrices forms a convex cone, the *copositive cone*  $\mathcal{COP}^n$ .

The matrix cone  $\mathcal{COP}^n$  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 [2], graph partitioning [3], computing the stability number [4], clique number [5], and chromatic number [6] of graphs, and the quadratic assignment problem [7]. Copositive formulations have been derived for quadratic programming problems [8, 9, 10] and mixed-integer programs [11]. For quadratically constrained quadratic programming problems with additional linear constraints copositive relaxations are tighter than standard Lagrangian semi-definite relaxations [12]. More applications of copositive programming can be found in the surveys [13, 14].

Verifying copositivity of a given matrix is a co-NP-complete problem [15]. Likewise, verifying whether a given linear hyperplane in the space  $\mathcal{S}^n$  of  $n \times n$  real symmetric matrices is supporting to  $\mathcal{COP}^n$  at the zero matrix is NP-hard [16]. Therefore much research has been focused on finding tractable approximations of the copositive cone, in particular, semi-definite approximations.

In [17] a hierarchy of inner semi-definite approximations for  $\mathcal{COP}^n$  has been constructed. In [10] this hierarchy has been relaxed to a hierarchy of polyhedral inner approximations.

For testing the quality of inner semi-definite approximations, and more generally algorithms for solving copositive programs, it is advantageous to use *extremal* copositive matrices, which are the hardest to approximate. An element  $x \in K$  is called *extremal* if a decomposition  $x = x_1 + x_2$  of  $x$  into elements  $x_1, x_2 \in \mathcal{COP}^n$  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*. 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. Since the extreme rays of  $\mathcal{COP}^n$  determine the facets

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of its dual cone, they are also important tools for the study of this dual cone, the completely positive cone [18, 19, 20, 21, 22, 23].

However, explicit families of non-trivial extremal copositive matrices or methods for their construction are relatively scarce [24, p.25], [25, Theorem 3.8], [26, 27, 28, 29, 30, 31, 32, 33]. Many of these are either discrete up to symmetry, or in a fixed low dimension.

In this paper we propose a method to construct multi-parametric families of extremal copositive matrices of arbitrary sizes. The main idea is to use result [34], which for every extremal copositive matrix  $A$  constructs an algebraic system of equations whose locus entirely consists of extremal copositive matrices in the neighbourhood of  $A$ . In general this system is difficult to solve. However, we show that for some of the matrices constructed in [32], namely the matrices obtained from COP-irreducible graphs with stability number 3, one may transform this system to a linear one by a trigonometric transformation. This allows to design an automated procedure to construct manifolds of extremal copositive matrices of arbitrary size.

We provide characteristics of the solution set for many examples (for graphs with up to 10 vertices) and a code to compute the solutions corresponding to arbitrary such graphs. We provide explicit examples of algebraic varieties of extremal copositive matrices with singularities.

For the cycle graph  $C_7$  we completely characterize the portion of the solution set which consists of copositive matrices, up to symmetries. It may be parameterized by 7 angle parameters varying in a polytope.

For further surveys on copositive matrices see [35, 36], for a list of open problems see [37].

The remainder of the paper is structured as follows. In Section 2 we provide auxiliary results which are useful later on. In Section 3 we provide the necessary background on copositive matrices obtained from COP-irreducible graphs. In Section 4 we construct the linear systems representing the algebraic varieties after a trigonometric transformation. In Section 5 we provide an analytic representation of the solution set around the matrix obtained from the cycle graph  $C_7$ . In the Appendix we present the solution set for some graphs with 8, 9, or 10 vertices.

## 2 Known results

### 2.1 Known extreme matrices family

As already mentioned in the introduction, the extreme rays of small dimensional copositive cones are completely characterized. There are algorithms that allow to construct an extreme ray of  $\mathcal{COP}^{n+1}$  from an extreme ray of  $\mathcal{COP}^n$ . One of them duplicates a row and the corresponding column [25, Theorem 3.8].

**Theorem 2.1.** *If  $Q_n$ ,  $n \geq 3$ , is an extreme copositive quadratic form in variables  $x_1, \dots, x_n$ , then replacing any  $x_i$  by  $x_i + x_{n+1}$  yields a new copositive form  $Q_{n+1}$  which is extreme.*

This allows in principle to obtain multi-parametric families of extreme copositive matrices in arbitrary dimension from a single such family in a given dimension.

In this paper we present another way to construct such families which does not rely on row and column duplication.

### 2.2 Irreducible matrices

In this section we introduce a concept which is slightly weaker than extremality.

The cone of copositive matrices  $\mathcal{COP}^n$  has the following two symmetry groups.

1. Permutation group:  $A \mapsto PAP^T, P \in S_n$
2. Group of positive definite diagonal matrices:  $A \mapsto DAD$

By the action of the second group any copositive matrix with positive diagonal elements can be scaled to a copositive matrix with all diagonal elements equal to 1.

**Definition 2.2.** For a matrix  $A \in \mathcal{COP}^n$  and a set  $\mathcal{M} \subset \mathcal{COP}^n$  we say that  $A$  is  $\mathcal{M}$ -irreducible if there do not exist  $\gamma > 0$  and  $M \in \mathcal{M} \setminus \{0_n\}$  such that  $A - \gamma M \in \mathcal{COP}^n$ .  $0_n$  here denotes a zero matrix.

**Lemma 2.3.** *Extremality and irreducibility with respect to the cone  $\mathcal{M} = \mathcal{S}_+^n + \mathcal{N}^n$  of positive semi-definite plus element-wise nonnegative matrices are invariant with respect to the action of the above-mentioned groups.*

*Proof.* • Let  $A \in \mathcal{COP}^n$  be extreme, then  $PAP^T$  is extreme too. Indeed, if there exist linearly independent  $B, C \in \mathcal{COP}^n$  such that  $PAP^T = B + C$ , then  $A = P^{-1}BP^{-T} + P^{-1}CP^{-T}$ , a contradiction. The reverse direction is proven similarly.

- For irreducibility the proof is similar. □

Thus we will not lose much if we restrict to the construction of extreme or/and irreducible matrices with all diagonal elements equal to 1.

### 2.3 Zeros and support sets

A useful characteristic of a copositive matrix  $A \in \mathcal{COP}^n$  are its minimal zeros, that is, non-zero vectors  $u \in \mathbb{R}_+^n$ , such that  $u^T A u = 0$  and there exists no other zero  $v$  of  $A$  with  $\text{supp}(v) \subset \text{supp}(u)$ . Here  $\text{supp}(u) = \{i | u_i > 0\}$  is the set of indices of non-zero elements of the vector. The following lemma [25, p. 200] holds for minimal zeros.

**Lemma 2.4.** *If  $u$  is a minimal zero of a copositive matrix  $A$ , then  $Au \geq 0$ .*

**Definition 2.5.** The complementary set of indices for a zero  $u$  of  $A \in \mathcal{COP}^n$  is the set of indices  $j$  such that  $(Au)_j = 0$ .

The extended minimal zero support set  $\mathcal{E} = \{(I_\alpha, J_\alpha)\}_{\alpha=1, \dots, m}$  of a matrix  $A$  is the set of pairs of supports  $I_\alpha$  of minimal zeros and the corresponding complementary sets  $J_\alpha$  of indices.

### 2.4 Trigonometric parametrization

The presence of zeros with supports of cardinality 3 allows to parameterize off-diagonal elements of the scaled matrix with all diagonal elements equal to 1 by angles.

The following result [33, Lemma 3] is a direct consequence of [38, Lemma 5.4 (e)] and [39, Lemma 4.7].

**Lemma 2.6.** *Let  $A \in \mathcal{COP}^n$  be a matrix with all diagonal elements equal to 1, let  $u \in \mathbb{R}_+^n$  be a minimal zero of  $A$  with support  $u = \{i, j, k\}$ . Then there exists a scalar  $\lambda > 0$  and angles  $\varphi_1, \varphi_2, \varphi_3 > 0$ , such that  $\varphi_1 + \varphi_2 + \varphi_3 = \pi$ ,  $(u_i, u_j, u_k) = \lambda(\sin \varphi_1, \sin \varphi_2, \sin \varphi_3)$  and  $A_{ij} = -\cos \varphi_3$ ,  $A_{ik} = -\cos \varphi_2$ ,  $A_{jk} = -\cos \varphi_1$ .*

We define a submatrix  $A_{\{a_1, \dots, a_k\}}$ , where  $1 \leq a_1 < a_2 < \dots < a_k \leq n$  as

$$A_{\{a_1, \dots, a_k\}} = \begin{pmatrix} A_{a_1, a_1} & A_{a_1, a_2} & \dots & A_{a_1, a_k} \\ A_{a_2, a_1} & A_{a_2, a_2} & \dots & A_{a_2, a_k} \\ \dots & \dots & \dots & \dots \\ A_{a_k, a_1} & A_{a_k, a_2} & \dots & A_{a_k, a_k} \end{pmatrix}$$

**Lemma 2.7.** *Let  $A \in \mathcal{COP}^n$  be a matrix with all diagonal elements equal to 1, let  $u, v \in \mathbb{R}_+^n$  be its minimal zeros with supports  $\text{supp}(u) = \{i, j, k\}$ ,  $\text{supp}(v) = \{j, k, l\}$ . Let the element  $l$  of the vector  $Au$  equal zero. Then there are positive  $\varphi_1, \varphi_2, \varphi_3$  such that  $\varphi_1 + \varphi_2 < \pi$ ,  $\varphi_2 + \varphi_3 < \pi$ , the submatrix  $A_{\{i, j, k, l\}}$  has the form*

$$\begin{pmatrix} 1 & -\cos(\varphi_1) & \cos(\varphi_1 + \varphi_2) & -\cos(\varphi_1 + \varphi_2 + \varphi_3) \\ -\cos(\varphi_1) & 1 & -\cos(\varphi_2) & \cos(\varphi_2 + \varphi_3) \\ \cos(\varphi_1 + \varphi_2) & -\cos(\varphi_2) & 1 & -\cos(\varphi_3) \\ -\cos(\varphi_1 + \varphi_2 + \varphi_3) & \cos(\varphi_2 + \varphi_3) & -\cos(\varphi_3) & 1 \end{pmatrix},$$

and in addition  $(Av)_i = 0$ .

*Proof.*

1. According to Lemma 2.6, we can parametrize  $A_{\text{supp}(u)}$  as

$$\begin{array}{c} i \\ j \\ k \end{array} \begin{array}{ccc} & i & j & k \\ \left( \begin{array}{ccc} 1 & -\cos \varphi_3 & -\cos \varphi_2 \\ -\cos \varphi_3 & 1 & -\cos \varphi_1 \\ -\cos \varphi_2 & -\cos \varphi_1 & 1 \end{array} \right) \end{array}$$

with  $u = \lambda(\sin \varphi_1, \sin \varphi_2, \sin \varphi_3)$ ,  $\varphi_1 + \varphi_2 + \varphi_3 = \pi$ . For  $A_{\text{supp}(v)}$  there exists a similar parametrization, where the coefficient  $A_{jk}$  is already known from the representation of the matrix  $A_{\text{supp}(u)}$ . We get for  $A_{\text{supp}(v)}$

$$\begin{array}{c} j \\ k \\ l \end{array} \begin{array}{ccc} & j & k & l \\ \left( \begin{array}{ccc} 1 & -\cos \varphi_1 & -\cos \varphi_4 \\ -\cos \varphi_1 & 1 & -\cos \varphi_5 \\ -\cos \varphi_4 & -\cos \varphi_5 & 1 \end{array} \right) \end{array}$$

with  $v = \lambda_1(\sin \varphi_4, \sin \varphi_5, \sin \varphi_1)$ ,  $\varphi_1 + \varphi_4 + \varphi_5 = \pi$ . Combining these two parametrizations, we obtain the following representation of  $A_{\{i,j,k,l\}}$  (see also [33, p. 164]):

$$\begin{array}{c} i \\ j \\ k \\ l \end{array} \begin{array}{cccc} & i & j & k & l \\ \left( \begin{array}{cccc} 1 & -\cos \varphi_3 & -\cos \varphi_2 & A_{i,l} \\ -\cos \varphi_3 & 1 & -\cos \varphi_1 & -\cos \varphi_4 \\ -\cos \varphi_2 & -\cos \varphi_1 & 1 & -\cos \varphi_5 \\ A_{i,l} & -\cos \varphi_4 & -\cos \varphi_5 & 1 \end{array} \right) \end{array}$$

2. We have  $\cos \varphi_2 = \cos(\pi - \varphi_1 - \varphi_3) = -\cos(\varphi_3 + \varphi_1)$  and  $\cos \varphi_4 = -\cos(\varphi_1 + \varphi_5)$ . By assumption  $(Au)_l = \lambda(A_{i,l} \sin \varphi_1 - \cos \varphi_4 \sin \varphi_2 - \cos \varphi_5 \sin \varphi_3) = 0$ , which yields

$$\begin{aligned} A_{i,l} \sin \varphi_1 &= \cos \varphi_5 \sin \varphi_3 - \cos(\varphi_1 + \varphi_5) \sin \varphi_3 + \varphi_1 \\ &= \cos \varphi_5 \sin \varphi_3 - \cos(\varphi_1 + \varphi_5) \cos \varphi_3 \sin \varphi_1 - \cos(\varphi_1 + \varphi_5) \sin \varphi_3 \cos \varphi_1 = \\ &= \sin \varphi_1 (\sin \varphi_3 \sin(\varphi_1 + \varphi_5) - \cos \varphi_3 \cos(\varphi_1 + \varphi_5)), \\ A_{i,l} &= -\cos(\varphi_1 + \varphi_3 + \varphi_5). \end{aligned}$$

We get a parametrization of the desired type, wherein  $\varphi_1 + \varphi_3 < \pi$ ,  $\varphi_1 + \varphi_5 < \pi$ , and all the angles are greater than 0.

3. Finally for the  $i$ -th component of  $Av$  we get

$$(Av)_i = \lambda_1(-\sin(\varphi_1 + \varphi_5) \cos \varphi_3 + \sin \varphi_5 \cos(\varphi_3 + \varphi_1) - \sin \varphi_1 \cos(\varphi_1 + \varphi_3 + \varphi_5)) = 0.$$

□

## 2.5 Cone stratification

Let us consider the cone stratification tool proposed in [34], which allows one to study the local structure of the boundary of the copositive cone and which is conveniently used to study its extreme rays. We shall need the following definition from convex analysis.

**Definition 2.8.** A convex set  $\mathcal{F} \subset \mathcal{COP}^n$  is called a *face* of  $\mathcal{COP}^n$  if for any closed segment  $l \subset \mathcal{COP}^n$  having at least one relative interior point in  $\mathcal{F}$ , both end points of  $l$  lie in  $\mathcal{F}$ .

The *minimal face*  $\mathcal{F}^A$  of the matrix  $A \in \mathcal{COP}^n$  is the intersection of all faces containing the matrix  $A$ .

For an extremal matrix  $A \in \mathcal{COP}^n$  we have  $\mathcal{F}^A = \{\lambda A \mid \lambda \geq 0\}$  by definition, i.e. for an extremal matrix, the minimum face has dimension 1.

Let us move on to the stratification method itself. The cone  $\mathcal{COP}^n$  can be partitioned into a disjoint union of sets  $S_{\mathcal{E}}$ . Here  $S_{\mathcal{E}}$  consists of matrices with extended minimal zero support set being equal to  $\mathcal{E}$ . In [34] it is shown that  $S_{\mathcal{E}}$  is locally an algebraic variety. More precisely, by introducing

$$Z_{\mathcal{E}} = \{A \in \mathcal{S}^n \mid A_{J_{\alpha} \times I_{\alpha}} \text{ has incomplete rank } \forall \alpha \in \{1, \dots, m\}\},$$

where  $\mathcal{S}^n$  is the space of  $n \times n$  real symmetric matrices, the following theorem holds [34, Theorem 1].

**Theorem 2.9.** *Let  $A \in \mathcal{COP}^n$ , let  $\mathcal{E} = \{(I_{\alpha}, J_{\alpha})\}_{\alpha=1, \dots, m}$  be the extended minimal zero support set of the matrix  $A$ . Then there exists a neighborhood  $U \subset \mathcal{S}^n$  of matrix  $A$  such that  $U \cap S_{\mathcal{E}} = U \cap Z_{\mathcal{E}}$ .*

This implies that in the neighborhood of any point the component  $S_{\mathcal{E}}$  is given by the solution set of a finite number of algebraic equations.

This extension method is convenient for studying extremal rays of the copositive cone due to the following lemma [34, Lemma 9].

**Lemma 2.10.** *Let  $\mathcal{E}$  be a set of pairs of indices, let  $C$  be an irreducible component of the algebraic variety  $Z_{\mathcal{E}}$ , such that  $S = S_{\mathcal{E}} \cap C \neq \emptyset$ . Then the dimension of the minimum face of the matrix  $A \in S$  is the same for all matrices of this set, possibly excluding a subset of lower dimension.*

An irreducible component of an algebraic set is an algebraic subset that cannot be decomposed into a union of two nontrivial algebraic subsets. It follows that if we take an extremal matrix, i.e., such that the dimension of the minimum face is equal to 1, almost all matrices in its component will have the same dimension of the minimal face, i.e., they will also be extreme.

In the next section we present a method to construct extremal copositive matrices using a specific graph family. This technique allows to construct discrete extremal rays of the copositive cone. The purpose of this paper is to extend them to a whole manifold of extreme rays.

### 3 COP-irreducible graphs and associated matrices

In [32] a method of construction of irreducible and extreme matrices using a special graph family was proposed. For all graphs  $G$  with adjacency matrix  $A_G$  the following matrix is copositive:

$$Z^G = \alpha(G)(I + A_G) - E,$$

where  $\alpha(G)$  is the stability number of  $G$  (the cardinality of its maximum stable sets), and  $E$  is the all-ones matrix. We have the following [32, Theorem 3]:

**Theorem 3.1.** *For a graph  $G$  we have that  $Z^G$  is irreducible with respect to  $\mathcal{S}_+^n + \mathcal{N}^n$  if and only if  $G$  is connected,  $\alpha$ -critical, and  $\alpha$ -covered.*

Here a graph is  $\alpha$ -critical if removing any edge will increase its stability number, it is  $\alpha$ -covered if for all  $(i, j) \in E(\overline{G})$  there exists a maximum stable set  $\mathcal{A}$  of  $G$  such that  $\{i, j\} \subseteq \mathcal{A}$ . In [32] graphs which are connected,  $\alpha$ -critical, and  $\alpha$ -covered are called COP-irreducible graphs.

Thus, to construct an irreducible matrix of dimension  $n$ , one may first take a COP-irreducible graph on  $n$  vertices, and then construct the corresponding matrix  $Z^G$ . For constructing matrices of arbitrary size some methods were proposed in [32]:

- Take an infinite family of COP-irreducible graphs. For example, antiwebs  $\overline{W}_t^n$ : graphs such that  $V(\overline{W}_t^n) = \{1, \dots, n\}$ ,  $E(\overline{W}_t^n) = \{ij : i < j < i + t, j < i + t - n\}$
- There are techniques for taking a COP-irreducible graph and constructing a larger COP-irreducible graph from this. For example, vertex duplication: take a graph  $G$  and a vertex  $v \in V(G)$ , then add a new vertex  $w$  and some edges:

$$H = E(G) + w + vw + \sum_{x: xv \in E(G)} xw$$

This method is suitable for construction of irreducible matrices. However, it is also established that almost every matrix constructed from a COP-irreducible graph on  $\leq 13$  vertices is extreme. Thus, the method is interesting also for constructing extremal copositive matrices.

We shall introduce the following notations. Let  $G$  be a COP-irreducible graph with stability number 3, and  $\mathcal{E}$  be the extended minimal zero support set of  $Z^G$ . Then we shall denote by  $S_G$  the set of matrices in the component  $S_{\mathcal{E}}$  which have all ones on the diagonal, and by  $Z_G$  the matrices in the algebraic variety  $Z_{\mathcal{E}}$  which have all ones on the diagonal. Then  $Z^G \in S_G \subset Z_G$ , and if  $Z^G$  is extremal, then  $S_G$  also consists of extremal matrices near  $Z^G$ . In the next section we shall describe an algorithm to compute  $Z_G$  explicitly.

## 4 Construction of linear systems

For a COP-irreducible graph  $G$  the corresponding matrix  $Z^G$  lies in some component  $S_{\mathcal{E}}$ . In this section we show that for stability number  $\alpha(G) = 3$ , the corresponding algebraic variety  $Z_G$  is described by linear relations on the angles parameterizing the matrices in  $Z_G$ , and construct the linear systems on these angles.

First let us take a COP-irreducible graph  $G = (V, E)$ ,  $V = \{1, \dots, n\}$  with a stability number  $\alpha(G) = 3$ . Dividing each row by 2 we get that the corresponding copositive matrix  $Z^G$  looks as follows:

$$Z_{ij}^G = \begin{cases} 1, & (i, j) \in E \\ 1, & i = j \\ -\frac{1}{2}, & (i, j) \notin E \end{cases}$$

The extended minimal zero support set of this matrix is clearly connected to the structure of the graph's stable sets. The following lemma is proved in the above-mentioned paper [32, Lemma 6].

**Lemma 4.1.** *The set  $I$  is a minimal zero support set of the matrix  $Z^G$  if and only if  $I$  is a maximal stable set of the graph  $G$ . Further, let  $u$  be a minimal zero of  $Z^G$  and  $l \notin \text{supp } u$ . Then the following conditions are equivalent:*

- $(Z^G u)_l = 0$
- exactly one pair of vertices  $(i, l)$  with  $i \in \text{supp } u$  is connected by an edge in  $G$ .

We get that the extended minimal zero support set of the matrix  $Z^G$  can be described in terms of the graph  $G$ . We further go on to describe the structure of the set  $S_G$ , the set of copositive matrices with all diagonal elements being equal to 1 and having the same extended minimal zero support set as  $Z^G$ .

**Lemma 4.2.** *Let  $G = (V, E)$  be a COP-irreducible graph with stability number 3, and let  $A \in S_G$ . Then every off-diagonal element  $A_{ij}$  can be represented as  $-\cos \varphi_{ij}$ , where  $\varphi_{ij} \in (0, \pi)$  for  $(i, j) \notin E$  and  $\varphi_{ij} \in (0, 2\pi)$  for  $(i, j) \in E$ .*

*Proof.* • If we take  $A_{ij}$  such that  $(i, j) \notin E$  then because of  $\alpha$ -coveredness of the graph  $G$  the vertices  $i, j$  should belong to some maximal stable set. Therefore they belong to some minimal zero support set of cardinality 3. Then such an angle exists by Lemma 2.6.

- If  $(i, j) \in E$  then because of  $\alpha$ -criticality there should exist a subgraph on 4 vertices in which  $(i, j)$  is the only edge, therefore we can use Lemma 2.7 to find the angle.

□

Each matrix  $A \in S_G$  is symmetric with all 1 diagonal, therefore we need just  $\frac{n(n-1)}{2}$  angles to describe it. Introduce a parameter vector of angles  $\bar{\varphi} \in \mathbb{R}^{\frac{n(n-1)}{2}}$  and a matrix function

$$A(\bar{\varphi}) = \begin{pmatrix} 1 & -\cos \varphi_1 & \cdots & -\cos \varphi_{n-1} \\ -\cos \varphi_1 & 1 & \cdots & -\cos \varphi_{2n-3} \\ \vdots & \vdots & \ddots & \vdots \\ -\cos \varphi_{n-1} & -\cos \varphi_{2n-3} & \cdots & 1 \end{pmatrix} \quad (1)$$

The relationship between an angle with one index and one with two indices is as follows:

$$\varphi_{ij} = \varphi_k, \quad k(i,j) = j + (i-1) \cdot n - \frac{i(i+1)}{2}, \quad \forall 1 \leq i < j \leq n$$

Now we can reformulate the previous lemma as follows.

**Corollary 4.3.** *Assume the conditions of Lemma 4.2. Then there exists a subset  $O_G \subset \mathbb{R}^{\frac{n(n-1)}{2}}$  such that  $A[O_G] = S_G$ .*

Here we denote  $A[O_G] = \{A(\bar{\varphi}) \mid \bar{\varphi} \in O_G\}$ .

This set is never empty: if we take the angles  $\varphi_{ij} = \begin{cases} \frac{\pi}{3}, & (i,j) \notin E \\ \pi, & (i,j) \in E \end{cases}$  and assemble a corresponding

vector  $\bar{\varphi}_0$ , then we get that  $A(\bar{\varphi}_0) = Z^G$ . The hope for this set  $O_G$  to have a simple description led to this research. We will spend the rest of the paper constructing this set for one graph and finding weaker results for all COP-irreducible graphs with  $\alpha(G) = 3$ .

Lemmas 2.6 and 2.7 not only prove the existence of parameter angles but also provide certain conditions that they must satisfy.

### Conditions from Lemma 2.6

From this lemma we get conditions on the elements that correspond to minimal zeros. From Lemma 4.1 we obtain that the minimal zero support sets coincide with the maximal stable sets of the graph  $G$ . We will call the collection of these sets  $SS(G)$ . Combining these facts we get the following conditions:

$$\begin{aligned} \forall \{i,j,k\} \in SS(G) &\Rightarrow \varphi_{ij} + \varphi_{jk} + \varphi_{ik} = \pi \\ 0 &< \varphi_{ij}, \varphi_{jk}, \varphi_{ik} < \pi \end{aligned}$$

We will write the first group of conditions as a system of linear equations:  $A_1 \bar{\varphi} = b$ , where  $b$  is a vector where all components are equal to  $\pi$ .

### Conditions from Lemma 2.7

From this lemma we get conditions on the angles  $\varphi_{ij}$  such that there exist minimal zeros with support sets  $\{i,k,l\}$  and  $\{j,k,l\}$  for some  $k,l$  distinct from  $i,j$ . From Lemma 4.1 we know that these pairs  $(i,j)$  are exactly the edges of the graph. Then for every  $(i,j) \in E$  and every  $k,l \in V$  such that  $\{i,k,l\}, \{j,k,l\} \in SS(G)$  we get:

$$-\cos \varphi_{ij} = -\cos(\varphi_{ik} + \varphi_{kl} + \varphi_{jl}) \Leftrightarrow \varphi_{ij} = \pi \pm (\varphi_{ik} + \varphi_{kl} + \varphi_{jl} - \pi) \Leftrightarrow \begin{cases} \varphi_{ij} = \varphi_{ik} + \varphi_{kl} + \varphi_{jl} \\ \varphi_{ij} = 2\pi - (\varphi_{ik} + \varphi_{kl} + \varphi_{jl}) \end{cases} \quad (2)$$

As we can see, for each angle corresponding to an edge two linear conditions are possible: one with the plus sign and one with minus. If we fix one choice of all signs then the conditions imposed by Lemma 2.7 are a set of linear equations.

Note that  $2\pi - (\varphi_{ik} + \varphi_{kl} + \varphi_{jl}) = \varphi_{il} + \varphi_{kl} + \varphi_{jk}$  by the conditions imposed by Lemma 2.6, i.e., exchanging  $k,l$  is equivalent to choosing the opposite sign in (2). We shall therefore specify the sign always together with the triple of angles  $\varphi_{ik}, \varphi_{kl}, \varphi_{jl}$ . In the tables in the Appendix the angles in this triple are listed in their single-indexed version.

For any given combination of signs used in the equations on  $\varphi_{ij}$ ,  $(i,j) \in E$ , the system of linear equalities and inequalities on the angles yields a solution set in angle space. We shall refer to such a combination by an *opening*, denoted  $o$ , to the corresponding solution set by  $U_o$ , and to the set of all combinations by  $\mathcal{O}$ .

For every  $(i,j) \in E$ , there exists a number  $N_{ij}$  of pairs  $(k,l) \notin E$  as above. For every such pair, fix a triple  $\varphi_{ik}, \varphi_{kl}, \varphi_{jl}$  of angles. Then we may associate the choice in the corresponding equation (2) to a sign  $\pm 1$ . Denote this sign by  $o \cdot \varphi_{ij}[r]$ , or  $o \cdot \varphi_m[r]$  in the equivalent single-indexed version of the angle, where  $r \in \{1, \dots, N_{ij}\}$  is the number of the pair  $(k,l)$ . The opening  $o$  then consists of blocks  $o \cdot \varphi_{ij}$ , each block consisting of  $N_{ij}$  signs.

In tables from Appendix we use the following format to describe our openings:

$$k_0(i,j) : \quad [([k_0(i,l), k_0(l,m), k_0(j,m)] : c(i,j,l,m)), \quad \forall l,m : \{i,l,m\}, \{j,l,m\} \in SS(G)] \quad (i,j) \in E$$



where  $c(i,j,l,m) \in \{1, -1\}$  and it shows which linear equation we are using:  $\varphi_{k(i,j)} = \pi + c(i,j,l,m) \cdot (\varphi_{k(i,l)} + \varphi_{k(l,m)} + \varphi_{k(j,m)} - \pi)$ ,  $k_0(i,j) = k(i,j) - 1$  - we have to subtract one from the vector index because indexing used in our software starts from 0.

For each opening the equality relations from Lemma 2.7 can be collected into a linear system  $A_o \bar{\varphi} = b_o$ , where the coefficient matrix and the right-hand side now depend on  $o$ .

**Lemma 4.4.** *For any opening  $o$ , the solution set  $U_o$  is mapped by the map (1) to an analytic manifold.*

*Proof.* The conditions on the angles amount to linear equalities and strict linear inequalities. Since the angles are bounded, the solution set  $U_o$  is a relatively open polytope in angle space. Moreover, the angles  $\varphi_{ij}$ ,  $(i,j) \in E$  are explicit linear functions of the remaining angles. But these remaining angles vary in the interval  $(0,\pi)$  on which the cosine is strictly monotone. Hence map (1) is analytic and invertible on the solution set, and its image is an analytic manifold.  $\square$

The dimension of this manifold is equal to the dimension of the polytope, and hence to the dimension of the affine subspace determined by the equality relations on the angles. Note that  $\bar{\varphi}_0 \in U_o$  for all  $o$ , so the manifolds all contain the central matrix  $Z^G$ .

*Remark 4.5.* If the angles  $\varphi_{kl}$ ,  $(k,l) \notin E$  are given, then the image  $A(\bar{\varphi})$  is uniquely determined, because the element  $A_{ij} = -\cos \varphi_{ij}$  for  $(i,j) \in E$  does not depend on the choice of the opening. However, different openings may still lead to different manifolds in matrix space, because the relations determining the angles  $\varphi_{ij}$ ,  $(i,j) \in E$  may imply additional linear equality constraints on the angles  $\varphi_{kl}$ ,  $(k,l) \notin E$ , and these can be dependent on the opening  $o$ .

Now we can view the non-linear conditions imposed on the entries of  $A$  by the lemmas as a union of linear systems on the angles  $\bar{\varphi}$  corresponding to different openings. Combining these conditions we get that our angles should lie in the following set:

$$\begin{aligned} U_G &= \{\bar{\varphi} : A_1 \bar{\varphi} = b\} \cap \bigcup_{o \in \mathcal{O}} \{\bar{\varphi} : A_o \bar{\varphi} = b_o\} \cap \{0 < \varphi_{ij} < \pi, (i,j) \notin E\} \cap \{0 < \varphi_{ij} < 2\pi, (i,j) \in E\} = \\ &= \bigcup_{o \in \mathcal{O}} \left\{ \{\bar{\varphi} : B_o \bar{\varphi} = c_o\} \cap \{0 < \varphi_{ij} < \pi, (i,j) \notin E\} \cap \{0 < \varphi_{ij} < 2\pi, (i,j) \in E\} \right\} = \bigcup_{o \in \mathcal{O}} U_o \\ &\quad B_o = \begin{bmatrix} A_1 \\ A_o \end{bmatrix}, \quad c_o = \begin{bmatrix} b \\ b_o \end{bmatrix} \end{aligned}$$

Thus the set  $U_G$  is a union of relatively open polytopes with the following properties:

**Lemma 4.6.** *Let  $G$  be a COP-irreducible graph with stability number 3, and  $U_G$  be the set in which the parametrization angles must lie. Then*

$$S_G \subseteq A[U_G] \tag{3}$$

*Proof.* The assertion follows from Lemmas 2.6 and 2.7.

However, not for every element in  $\bar{\varphi} \in U_G$  the matrix  $A(\bar{\varphi})$  is necessarily an element of  $S_G$ . Some of the matrices might not be copositive or might have additional elements in their extended minimal zero support set.  $\square$

## 4.1 Determining smoothness and dimension of $S_G$

The set  $U_G$  can be used to derive some fundamental properties of the  $S_G$  variety. We have the following connection:

**Lemma 4.7.**  $\exists o \in \mathcal{O} : U_G = U_o \Leftrightarrow S_G$  is a smooth set and  $\dim(U_G) = \dim(S_G)$

*Proof.* This is a direct consequence of Lemma 4.4.  $\square$

If there is no such opening then  $U_G$  is a union of polytopes and their common points are points of singularity.

So to determine smoothness of set  $S_G$  we need to find whether there exists an opening  $o_{base} \in \mathcal{O}$  such that  $U_o \subseteq U_{o_{base}} \forall o \in \mathcal{O}$ . Since all of the sets lie in the same  $(0, \pi)$  cube and all of them share at least one point  $\bar{\varphi}_0$  in common, this condition comes down to finding  $o_{base}$  such that  $Ker(B_0) \subseteq Ker(B_{o_{base}}) \forall o \in \mathcal{O}$ .

The simplest algorithm to find such an opening would be to build the constraint systems  $B_o$  for all openings  $o$ , compute the basis of their kernels, sort them in descending order by their dimension and then go linearly through it checking what spaces can not be embedded into previous ones. But this algorithm would be too expensive even for small graphs. Below we propose a couple of improvements to check graphs with at least 11 vertices on a personal computer.

First we don't need to check all of the openings because some of them correspond to the same set of matrices.

**Lemma 4.8.** *Let  $o_1, o_2 \in \mathcal{O}$  be two openings such that for each  $(i, j) \in E$  we have either  $o_1.\varphi = o_2.\varphi$  or  $o_1.\varphi = -o_2.\varphi$ . Then  $A(U_{o_1}) = A(U_{o_2})$ , i.e., the openings yield the same manifold.*

*Proof.* The solution set  $U_{o_2}$  can be obtained from the solution set  $U_{o_1}$  by the transformations  $\varphi_{ij} \mapsto \begin{cases} \varphi_{ij} \\ 2\pi - \varphi_{ij} \end{cases}$ , depending on whether  $o_1.\varphi_{ij} = o_2.\varphi_{ij}$  or  $o_1.\varphi_{ij} = -o_2.\varphi_{ij}$ . This has, however, no impact on the values of  $A_{ij} = -\cos \varphi_{ij}$ .  $\square$

This allows us to reduce the number of openings that we have to check by a factor of  $2^{|E|}$ :

**Corollary 4.9.**  $U_G = \bigcup_{o \in \bar{\mathcal{O}}} U_o$ ,  $\bar{\mathcal{O}} = \{o \in \mathcal{O} : \forall \varphi o.\varphi[1] = 1\}$

A further improvement of the straight-forward algorithm is not to store a basis of the subspaces but to compute them on the fly. By combining these two ideas we get Algorithm 4.1 to determine the smoothness and dimensionality of  $S_G$ .

---

**Algorithm 1** Algorithm to determine smoothness and dimensionality of  $S_G$

---

```

BS ← ∅      ▷ An array of "basic" subspaces that we keep sorted by the dimensionality of their kernel.
for o ∈  $\bar{\mathcal{O}}$  do
  cp ← 1
                ▷ We check if the new subspace can be embedded into the ones in the "basic" array.
  while cp < len(BS) and dim(Ker(BS[cp])) ≥ dim(Ker(Bo)) do
    if Ker(Bo).is_subspace(Ker(BS[cp])) then return
    end if
    cp ← cp + 1
  end while
  ▷ We either came to the end of the array or subspaces after position cp have smaller dimension than the
  current one
  BS.insert(Bo, cp)
  ▷ Now we need to check whether the subspaces of smaller dimension are embedded into the new one.
  while cp < len(BS) do
    if Ker(BS[cp]).is_subspace(Ker(Bo)) then
      BS.pop(cp)
    end if
    cp ← cp + 1
  end while
end for

```

---

If after running the algorithm we have only one subspace in the array  $BS$ , then  $S_G$  is smooth and  $\dim(S_G) = \dim(BS[1])$ . If there is more than one subspace then the variety  $Z_G$  contains a singularity at  $Z^G$ . The *is\_subspaces* function just concatenates two matrices and checks whether the rank of the concatenation is the same as the rank of the matrix that corresponds to the ambient space. We compute the rank of the matrix by the standard matlab function that uses a singular value decomposition and checks the number of non-zero singular values.

A code for this algorithm can be found in our repository [40]. In the table in Section 8 we provide examples of graphs which correspond to smooth components  $S_G$ .

The varieties corresponding to some graphs turn out to have singular points. We describe one such graph in the next section.

## 4.2 Components with singularity

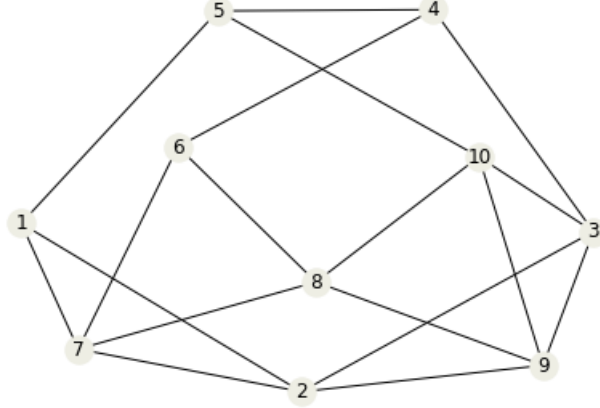


Figure 1: Example of a graph corresponding to a singular component

Not in all cases the conditions on the angles  $\bar{\varphi}$  for the matrix  $A(\bar{\varphi})$  to belong to a component  $Z_G$  define a polytope. Consider for example the graph in Fig. 1. The component corresponding to it has the following structure of the extended minimal zero support set:

$$\mathcal{I} = [[1, 3, 6], [1, 3, 8], [1, 4, 8], [1, 9, 4], [1, 10, 4], [1, 9, 6], [1, 10, 6], [2, 4, 8], [2, 4, 10], [2, 5, 6], [2, 5, 8], [2, 6, 10], [3, 5, 6], [3, 5, 7], [3, 5, 8], [9, 4, 7], [10, 4, 7], [9, 5, 6], [9, 5, 7]]$$

$$\begin{aligned} \mathcal{J} = & [[1, 3, 5, 6, 8, 9, 10], [1, 3, 4, 5, 6, 8], [1, 2, 3, 4, 8, 9, 10], [1, 4, 6, 7, 8, 9, 10], \\ & [1, 2, 4, 6, 7, 8, 9, 10], [1, 3, 4, 5, 6, 9, 10], [1, 2, 3, 4, 6, 9, 10], [1, 2, 4, 5, 8, 10], \\ & [1, 2, 4, 6, 7, 8, 10], [2, 3, 5, 6, 8, 9, 10], [2, 3, 4, 5, 6, 8], [1, 2, 4, 5, 6, 10], \\ & [1, 2, 3, 5, 6, 7, 8, 9], [3, 5, 6, 7, 8, 9], [1, 2, 3, 5, 6, 7, 8], [1, 4, 5, 7, 9, 10], \\ & [1, 2, 4, 7, 9, 10], [1, 2, 3, 5, 6, 7, 9], [3, 4, 5, 6, 7, 9]] \end{aligned}$$

In order to describe the structure of the component, we shall temporarily change the restrictions  $(Au)_l = 0$  associated with the complementary sets of the zeros with supports  $\{2,4,8\}$ ,  $\{2,5,8\}$ ,  $\{4,7,9\}$ ,  $\{5,7,9\}$ , and pass to larger components  $S_{\mathcal{E}}$  (or more precisely, their intersections with the all-ones diagonal subspace). Instead of demanding equality, we shall demand the conditions  $(Au_{248})_5 = (Au_{258})_4 > 0$  and  $(Au_{479})_5 = (Au_{579})_4 > 0$ . This corresponds to removing the index 4 from  $J_{11}$  and  $J_{19}$  and the index 5 from  $J_8$  and  $J_{16}$ . Recall that the inequality cannot be in the opposite direction without violating the copositivity of  $A$ .

Let us also shift the angles by an affine transformation, introducing parameters  $a_1, \dots, a_9$ , such that the matrix components  $A_{ij}$  are parameterized as in (5) in the Appendix. Then the central point  $Z^G$  is obtained by setting all parameters equal to zero.

The new inequalities impose the following restrictions on the angle  $\varphi_{45}$ , or equivalently, the parameter  $a_9$ :

$$\cos(\pi \cdot (1 - a_7 - a_8)) > \cos(\pi \cdot (1 - a_9)), \quad \cos(\pi \cdot (1 + a_7 - a_8)) > \cos(\pi \cdot (1 - a_9)).$$

In the neighbourhood of the central point  $a_7 = a_8 = a_9 = 0$  this can be equivalently written as

$$|a_9| < |a_7 + a_8|, \quad |a_9| < |a_8 - a_7|.$$

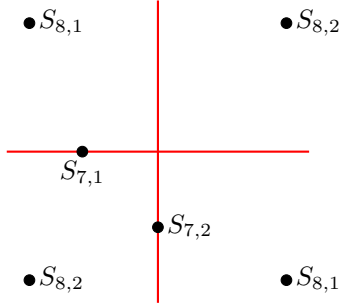


Figure 2: Components  $S_{8,1}, S_{8,2}$  in the parameter plane of  $a_7, a_8$ . The cross corresponds to the singular variety  $Z_G$ , with the singularity in the central point.

Thus, we have obtained a 9-dimensional component  $S_9$ , whose parameters  $a_1, \dots, a_8$  take any values near the central point, and for the last parameter we have

$$A_{45} = -\cos(\pi(1 - a_9)) > \max(-\cos(\pi \cdot (1 - a_7 - a_8)), -\cos(\pi \cdot (1 + a_7 - a_8))).$$

Enforcing one of the two equality constraints  $(Au_{248})_5 = (Au_{258})_4 = 0$  or  $(Au_{479})_5 = (Au_{579})_4 = 0$  individually, we get two smaller components  $S_{8,1}, S_{8,2}$  of dimension 8, for which the parameter  $a_9$  obeys

$$|a_9| = |a_7 + a_8|$$

or

$$|a_9| = |a_8 - a_7|,$$

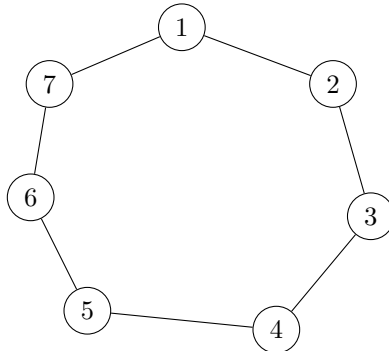
respectively. In addition we have the remaining inequality constraint, for  $S_{8,1}$   $|a_7 + a_8| < |a_8 - a_7|$  and for  $S_{8,2}$   $|a_8 - a_7| < |a_7 + a_8|$ . In Fig. 2 the corresponding loci for the pairs  $(a_7, a_8)$  are depicted. We see that the areas are not connected.

The component  $S_G$  is located on the intersection of the boundaries of  $S_{8,1}, S_{8,2}$ , where all the inequalities considered above are equalities. However, the equality  $|a_7 + a_8| = |a_8 - a_7|$  is equivalent to  $a_7 a_8 = 0$ , which factorizes in two different linear equations on the parameters. These correspond to two different manifolds which are the images of different polytopes in angle space. In the  $a_7, a_8$  parameter plane the manifolds correspond to the horizontal and the vertical line in Fig. 2. We shall denote these two 7-dimensional components by  $S_{7,1}, S_{7,2}$ . We stress that they both belong to the same variety  $Z_G$ . However, this variety presents a singularity at  $Z^G$ .

More examples of graphs defining a component with a singularity are given in the table in Section 9, examples corresponding to smooth extensions as in Lemma 4.7 are given in the table in Section 8 of the Appendix.

## 5 Case of cycle graph $C_7$

A cycle graph with 7 vertices, denoted  $C_7$ , is COP-irreducible [32] and  $\alpha(C_7) = 3$ . We may then apply the results developed in the previous section to compute the corresponding component  $S_{C_7}$ .



(4)



*Proof.*

$\Rightarrow$ : was shown above.

$\Leftarrow$ : It is necessary to show that for all angles from the described polytope the corresponding matrices  $A(\bar{\varphi})$  will be copositive, with the same extended minimal zero support set as  $Z^{C\tau}$ , i.e. it is in the component  $S_{C\tau}$ .

To show that the matrices are copositive we consider all subsets  $\mathcal{I}$  of  $\mathbb{P}[n]$  and either show that the submatrix  $A_{\mathcal{I}}$  is copositive, or present a corresponding certificate  $\mathbf{u}$  of copositivity. For simplicity we shall sometimes present the shorter subvector  $u_{\mathcal{I}}$ , since  $u_i$  for  $i \notin \mathcal{I}$  have to be zero anyway.

- For a subset of size 1 and 2, the certificate  $\mathbf{u} = \mathbf{e}_{\mathcal{I}} = \sum_{i \in \mathcal{I}} \mathbf{e}_i$  can be taken.
- For subsets of size 3:
  - If the set coincides with the support of some minimal zero, then this minimal zero itself will be a certificate.
  - $\{1,3,7\}$ : Since the corresponding submatrix of  $A$  is singular matrix, we have

$$\begin{pmatrix} 1 & -\varphi_1 & -(\varphi_1 + \varphi_2 + \varphi_3) \\ -\varphi_1 & 1 & (\varphi_2 + \varphi_3) \\ -(\varphi_1 + \varphi_2 + \varphi_3) & (\varphi_2 + \varphi_3) & 1 \end{pmatrix} \begin{pmatrix} \sin(\varphi_2 + \varphi_3) \\ \sin(\varphi_1 + \varphi_2 + \varphi_3) \\ -\sin \varphi_1 \end{pmatrix} = 0$$

and the vector above can be taken as a certificate.  $\{1,3,4\}$  is analyzed in similar way.

- $\{1,3,2\}$ : From Lemma 2.4 follows

$$\cos(\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4) + \cos(\varphi_5 + \varphi_6 + \varphi_7) < 0 \Rightarrow$$

$$\exists t > 0 : -\cos(\varphi_5 + \varphi_6 + \varphi_7) = \cos(\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4) + t.$$

Then we can represent the submatrix as a sum of two matrices, one of which has non-negative elements, and the other is copositive. Hence the submatrix

$$\begin{pmatrix} 1 & -\varphi_1 & (\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4) \\ -\varphi_1 & 1 & -(\varphi_2 + \varphi_3 + \varphi_4) \\ (\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4) & -(\varphi_2 + \varphi_3 + \varphi_4) & 1 \end{pmatrix} + E_{1,3}t = A_{(1,3,2)}$$

will also be copositive. Here  $E_{i,j}$  is a matrix which has zero entries everywhere except at  $(i,j)$  and  $(j,i)$ , where the entries equal 1. To prove the copositivity of the first term, we take a certificate similar to the previous case. Hence the matrix  $A_{(1,3,2)}$  is copositive.  $\{1,5,2\}$  is analyzed in similar way.

- The remaining subsets are obtained by a cyclic shift of those considered.
- For subsets of size 4:
  - If the set of matrix indices includes the minimal zero support, then the minimal zero could be taken as a certificate.  $Au \geq 0$  will imply that this is a certificate.
  - $\{1,3,7,2\}$ :  
We have

$$\begin{pmatrix} 1 & (\varphi_2 + \varphi_3) & -(\varphi_2 + \varphi_3 + \varphi_4) \\ (\varphi_2 + \varphi_3) & 1 & -\varphi_4 \\ -(\varphi_2 + \varphi_3 + \varphi_4) & -\varphi_4 & 1 \end{pmatrix} \begin{pmatrix} -\sin(\varphi_4) \\ \sin(\varphi_2 + \varphi_3 + \varphi_4) \\ \sin(\varphi_2 + \varphi_3) \end{pmatrix} = 0$$

Define the certificate  $u$  such that  $u_{(3,7,2)}$  equals the vector above. It remains to show that  $(Au)_1 \geq 0$ :

$$\sin \varphi_4 \cos \varphi_1 - \cos(\varphi_1 + \varphi_2 + \varphi_3) \sin(\varphi_2 + \varphi_3 + \varphi_4) - \cos(\varphi_5 + \varphi_6 + \varphi_7) \sin(\varphi_2 + \varphi_3) \geq 0$$

After simplifying:

$$\cos(\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4) + \cos(\varphi_5 + \varphi_6 + \varphi_7) \leq 0$$

And this is just one of the restrictions on the angles we received.

– {1,5,2,4}:

$$A = \begin{pmatrix} 1 & (\varphi_1 + \varphi_2) & -(\varphi_5 + \varphi_6 + \varphi_7) & (\varphi_6 + \varphi_7) \\ (\varphi_1 + \varphi_2) & 1 & (\varphi_3 + \varphi_4) & -(\varphi_3 + \varphi_4 + \varphi_5) \\ -(\varphi_5 + \varphi_6 + \varphi_7) & (\varphi_3 + \varphi_4) & 1 & -\varphi_5 \\ (\varphi_6 + \varphi_7) & -(\varphi_3 + \varphi_4 + \varphi_5) & -\varphi_5 & 1 \end{pmatrix}$$

Let's start with the simplest certificate  $u = (0, -\sin \varphi_5, \sin(\varphi_3 + \varphi_4 + \varphi_5), \sin(\varphi_3 + \varphi_4))^T$ . The  $Au$  components will then be non-negative if  $\cos(\varphi_1 + \varphi_2) + \cos(\varphi_3 + \dots + \varphi_7) \leq 0$ , i.e. for such angles we have provided a certificate.

Now consider the case when  $\cos(\varphi_1 + \varphi_2) + \cos(\varphi_3 + \dots + \varphi_7) > 0$ .

Further the notation will be used:

$$\begin{aligned} \cos(\varphi_1 + \varphi_2) &= -\cos(\varphi_3 + \dots + \varphi_7) + t_1 \\ \psi_1 &= \varphi_3 + \varphi_4, \quad \psi_2 = \varphi_6 + \varphi_7, \quad \psi_3 = \varphi_5 \end{aligned}$$

Then the submatrix can be represented as:

$$A_{(1,5,2,4)} = \begin{pmatrix} 1 & -(\psi_1 + \psi_2 + \psi_3) & -(\psi_2 + \psi_3) & \psi_2 \\ -(\psi_1 + \psi_2 + \psi_3) & 1 & \psi_1 & -(\psi_1 + \psi_3) \\ -(\psi_2 + \psi_3) & \psi_1 & 1 & -\psi_3 \\ \psi_2 & -(\psi_1 + \psi_3) & -\psi_3 & 1 \end{pmatrix} + E_{1,2}t_1$$

The first term can be transformed by permuting rows and columns, and then decomposing it into a product of two matrices as follows:

$$\begin{aligned} B &= \begin{pmatrix} 1 & \psi_2 & -(\psi_2 + \psi_3) & -(\psi_1 + \psi_2 + \psi_3) \\ \psi_2 & 1 & -\psi_3 & -(\psi_1 + \psi_3) \\ -(\psi_2 + \psi_3) & -\psi_3 & 1 & \psi_1 \\ -(\psi_1 + \psi_2 + \psi_3) & -(\psi_1 + \psi_3) & \psi_1 & 1 \end{pmatrix} = \\ &= \begin{pmatrix} \sin \psi_2 & \cos \psi_2 \\ 0 & 1 \\ \sin \psi_3 & -\cos \psi_3 \\ \sin(\psi_1 + \psi_3) & -\cos(\psi_1 + \psi_3) \end{pmatrix} * \begin{pmatrix} \sin \psi_2 & \cos \psi_2 \\ 0 & 1 \\ \sin \psi_3 & -\cos \psi_3 \\ \sin(\psi_1 + \psi_3) & -\cos(\psi_1 + \psi_3) \end{pmatrix}^T = U * U^T. \end{aligned}$$

Hence this matrix turns out to be positive semi-definite, and then the first term in the representation of  $A_{(1,5,2,4)}$  will also be positive semi-definite, hence  $A_{(1,5,2,4)}$  is copositive.

– The remaining subsets are obtained from the previous one by a cyclic permutation of the indices.

- Subsets of size 5,6,7: In this case, the sets will always include minimal zero supports, and then we can take the corresponding minimal zeros  $u$  as a certificate. From  $Au \geq 0$  we get that they fit the conditions.

Thus, we have shown that for any set of angles, for the corresponding matrix, one can give certificates of copositivity.  $\square$

## 6 Generation scheme

There is a different way to generate extreme matrices depending on the size  $n$  we need.

- $n = 7$ : Here we use Lemma 5.2 for a cycle graph: we take a vector of angles that satisfy the conditions of the lemma and construct the corresponding matrix  $A(\vec{\varphi})$ . This matrix will be copositive and since it belongs to the same variety as  $Z^{C_7}$  it will almost certainly be extreme because of Lemma 2.10.

- $8 \leq n \leq 12$ : The process here involves a couple of more steps:
  1. Take one of the graphs  $G$  for which we have precomputed the base opening in the table in Section 8. Then we take the basis given by the matrix  $B_o$ , generate a random direction  $\bar{r}$  lying in the matrix kernel.
  2. Then find a small enough scalar  $\alpha$  such that  $A(\bar{\varphi}_0 + \alpha\bar{r}) \in S_G$ . This can be done by decreasing  $\alpha$  from 1 to 0 and algorithmically checking copositivity and the extended minimal zero support set structure.
  3. By Lemma 2.10 the matrix is almost certainly extreme.
- $n > 12$ : Here another task we need to solve is to generate a COP-irreducible graph  $G$  with  $\alpha(G) = 3$  such that  $Z^G$  is an extreme matrix. There are multiple ways to do that:
  1. In [32, Lemma 11] it is shown that by using vertex duplication from a COP-irreducible graph we can get a COP-irreducible graph with the same  $\alpha(G)$ . Hence graphs with any number of vertices can be constructed from graphs in the table.
  2. From [32, Lemma 2] we get that by taking an antiweb  $\overline{W}_t^n$  with parameters  $t = k \in \mathbb{N} \setminus \{1\}$ ,  $n = 4k - 1$  we get a COP-irreducible graph with  $\alpha(\overline{W}_t^n) = 3$  with arbitrary large numbers of vertices.

To check that the graph corresponds to an extreme matrix we can use one of the algorithmic tests, e.g., [42, Theorem 17].

Now if you want to determine whether the variety is smooth or not you can use Algorithm 1 but it can be infeasible for graphs of medium size. If this fact isn't relevant to your research then you can take a random opening  $o$ . After getting a matrix  $B_o$  we repeat steps from the previous part.

Now we have generated an extreme copositive matrix with all ones on the diagonal, to go even further we can generate a random permutation matrix  $P$  and a diagonal matrix  $D$  to get an extreme matrix with a different diagonal. The fact the matrix would be extreme follows from Lemma 2.3.

## 7 Conclusion

There are two main contributions in this paper:

- An algorithm to generate a non-degenerate extreme copositive matrix of arbitrary dimension in generic position in a multi-parameter family.
- We have shown that the extended minimal zero support set varieties proposed in [34] can contain singular points.

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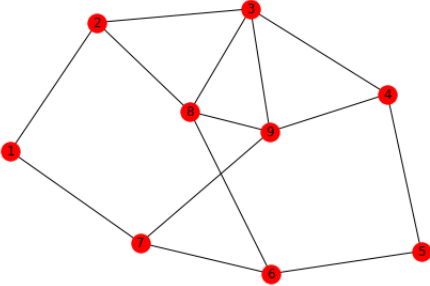
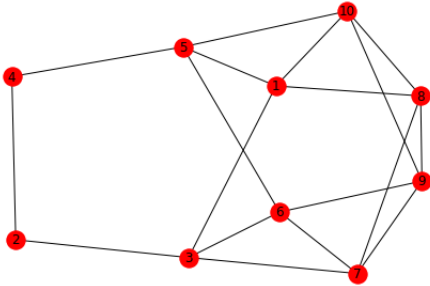
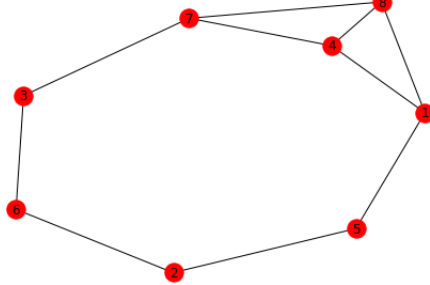
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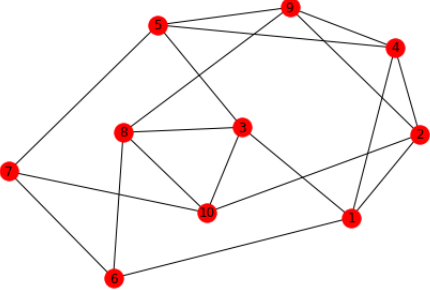
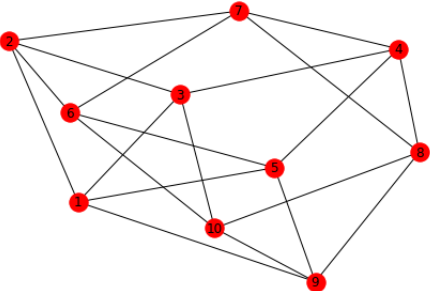
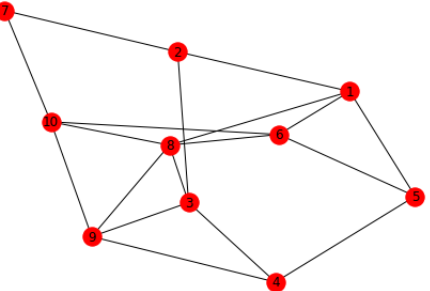
# Appendix

## 8 Examples of smooth components

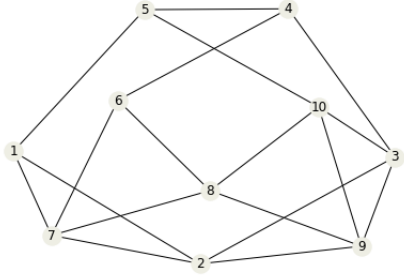
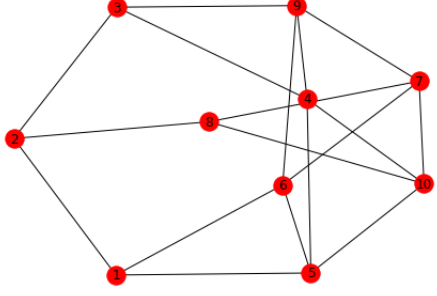
Here we present a part of the results in repository [40]. In file results.txt more are listed.

Graph	$\dim(S_G)$	Basic opening
	6	0: $[[2, 20, 11], 1]$ , 3: $[[1, 16, 23], 1]$ , 4: $[[1, 17, 26], 1], [2, 21, 26], 1]$ , 7: $[[9, 22, 15], 1], [9, 23, 16], 1]$ , 12: $[[8, 19, 26], 1]$ , 13: $[[1, 5, 20], 1], [1, 6, 21], 1]$ , $[15, 26, 21], 1]$ , 18: $[[8, 10, 22], 1], [8, 11, 23], 1]$ , 24: $[[14, 15, 26], 1]$ , 25: $[[10, 8, 20], 1], [10, 9, 23], 1]$ , $[15, 14, 23], 1]$ , 27: $[[5, 1, 17], 1], [5, 2, 21], 1]$
	8	0: $[[5, 33, 13], 1]$ , 2: $[[3, 27, 23], 1]$ , 4: $[[1, 16, 26], 1], [1, 19, 31], 1]$ , 8: $[[11, 31, 19], 1]$ , 10: $[[9, 22, 26], 1], [9, 23, 27], 1]$ , 15: $[[16, 26, 22], 1]$ , 18: $[[1, 3, 27], 1], [1, 6, 33], 1]$ , 24: $[[9, 11, 31], 1], [9, 12, 33], 1]$ , 28: $[[3, 1, 19], 1], [3, 5, 33], 1]$ , $[16, 17, 31], -1]$ , 29: $[[3, 1, 20], 1]$ , 30: $[[11, 9, 23], 1], [11, 13, 33], 1]$ , $[22, 21, 27], -1]$ , 32: $[[11, 9, 25], 1]$ , 34: $[[12, 9, 25], 1]$ , 35: $[[6, 1, 20], 1]$
	7	0: $[[2, 23, 12], 1], [3, 27, 12], 1]$ , 4: $[[1, 19, 31], 1], [2, 24, 31], 1]$ , 7: $[[1, 16, 29], 1]$ , 8: $[[14, 29, 16], 1], [14, 32, 17], 1]$ , 13: $[[9, 22, 31], 1]$ , 15: $[[1, 6, 24], 1], [17, 31, 24], 1]$ , 18: $[[1, 3, 27], 1]$ , 21: $[[2, 5, 27], 1], [9, 12, 27], 1]$ , 25: $[[9, 11, 32], 1]$ , 26: $[[29, 14, 11], 1], [29, 20, 17], 1]$ , 28: $[[3, 1, 19], 1]$ , 30: $[[11, 9, 23], 1]$ , 33: $[[5, 2, 24], 1]$ , 34: $[[12, 10, 29], 1]$ , 35: $[[19, 17, 32], 1]$

Graph	$\dim(S_G)$	Basic opening
	7	0: $[(2, 22, 11), 1], ([7, 29, 10], 1),$ $([7, 32, 11], 1),$ 5: $[(1, 16, 27), 1], ([2, 24, 33], -1),$ $([3, 28, 33], -1),$ 8: $[(10, 27, 18], 1),$ 13: $[(9, 23, 33], 1), ([10, 27, 33], 1),$ 15: $[(1, 4, 22], 1),$ 19: $[(1, 3, 28), 1], ([16, 27, 33], -1),$ 20: $[(1, 3, 29), 1], ([1, 4, 32], 1),$ 21: $[(2, 6, 28), 1], ([9, 12, 27], -1),$ $([23, 33, 28], 1),$ 25: $[(2, 4, 32], 1), ([9, 11, 32], 1),$ 26: $[(3, 1, 17], 1), ([3, 7, 32], 1),$ $([29, 14, 11], -1),$ 30: $[(11, 9, 23], 1),$ 31: $[(4, 2, 24], 1),$ 34: $[(12, 10, 29], 1),$ 35: $[(6, 3, 29), 1]$
	8	1: $[(7, 28, 17], 1),$ 3: $[(0, 13, 31], 1), ([7, 15, 11], -1),$ 6: $[(0, 12, 36], 1), ([2, 25, 36], 1),$ 8: $[(0, 12, 38], 1), ([0, 13, 41], 1),$ $([2, 25, 38], 1), ([2, 26, 41], 1),$ 9: $[(11, 32, 21], 1), ([15, 33, 18], -1),$ 10: $[(0, 4, 25], 1), ([0, 5, 26], 1),$ $([0, 7, 28], 1), ([12, 36, 27], -1),$ $([16, 38, 25], 1), ([16, 41, 26], 1),$ 19: $[(17, 27, 36], 1), ([23, 29, 25], -1),$ 20: $[(23, 29, 26], 1),$ 24: $[(17, 21, 32], 1), ([28, 22, 18], -1),$ 30: $[(11, 14, 36], 1),$ 34: $[(11, 13, 41], 1),$ 35: $[(4, 0, 13], 1), ([4, 2, 26], 1),$ $([12, 16, 41], -1), ([38, 29, 26], 1),$ 37: $[(4, 0, 15], 1), ([4, 2, 28], 1),$ 39: $[(13, 11, 32], 1),$ 40: $[(5, 0, 15], 1), ([5, 2, 28], 1),$ $([13, 11, 33], -1),$ 42: $[(14, 11, 33], 1), ([21, 17, 28], 1),$ $([21, 18, 33], 1),$ 43: $[(14, 12, 38], 1), ([21, 17, 29], -1),$ $([27, 25, 38], 1),$ 44: $[(22, 17, 29], 1)$
	8	2: $[(0, 7, 13], 1),$ 3: $[(4, 25, 23], 1),$ 6: $[(0, 7, 17], 1),$ 9: $[(7, 13, 18], 1), ([7, 17, 24], 1),$ 10: $[(0, 5, 25], 1),$ 15: $[(13, 18, 22], 1), ([14, 24, 26], -1),$ 16: $[(1, 0, 11], 1),$ 20: $[(18, 22, 25], 1),$ 21: $[(8, 7, 17], 1), ([13, 14, 24], -1),$ $([18, 22, 26], 1),$ 27: $[(23, 22, 26], 1)$

Graph	$\dim(S_G)$	Basic opening
	8	0: $[[[3, 32, 14], 1], ([5, 39, 14], 1)],$ 1: $[[[7, 40, 20], 1)],$ 2: $[[[5, 39, 27], 1)],$ 4: $[[[8, 34, 30], 1], ([7, 44, 38], -1)],$ 10: $[[[9, 19, 25], 1], ([9, 20, 26], 1),$ $[[13, 39, 27], -1)],$ 15: $[[[9, 19, 37], 1], ([9, 20, 40], 1)],$ 16: $[[[11, 30, 38], 1)],$ 18: $[[[9, 12, 30], 1)],$ 21: $[[[9, 13, 39], 1], ([17, 26, 39], 1)],$ 23: $[[[17, 25, 38], 1], ([22, 37, 38], 1)],$ 24: $[[[29, 38, 30], 1)],$ 28: $[[[17, 19, 37], 1], ([17, 20, 40], 1),$ $[[29, 38, 37], 1)],$ 31: $[[[3, 6, 39], 1], ([11, 14, 39], 1)],$ 33: $[[[3, 8, 44], 1], ([34, 38, 37], -1)],$ 35: $[[[12, 9, 20], 1], ([19, 17, 26], -1),$ $[[37, 22, 20], 1)],$ 36: $[[[12, 11, 32], 1)],$ 41: $[[[5, 7, 44], 1)],$ 42: $[[[6, 5, 40], 1)],$ 43: $[[[6, 3, 34], 1)]$
	10	0: $[[[8, 29, 10], 1], 1: [[4, 36, 21], 1)],$ 3: $[[[8, 41, 31], 1)], 7: [[2, 25, 37], 1)],$ 9: $[[[11, 32, 21], 1)], 12: [[15, 28, 25], 1)],$ 13: $[[[16, 34, 31], 1)], 17: [[22, 37, 25], 1)],$ 23: $[[[18, 31, 41], 1)], 24: [[10, 16, 34], 1)],$ 26: $[[[2, 8, 41], 1)], 27: [[2, 4, 36], 1)],$ 30: $[[[18, 21, 36], 1)], 33: [[18, 20, 40], 1)],$ 35: $[[[37, 22, 20], 1)], 38: [[4, 2, 29], 1)],$ 39: $[[[20, 18, 32], 1)], 42: [[21, 19, 37], 1)],$ 43: $[[[14, 11, 34], 1)], 44: [[15, 10, 29], 1)]$
	7	0: $[[[8, 29, 10], 1)],$ 3: $[[[1, 20, 31], 1], ([8, 23, 18], -1),$ $[[7, 40, 31], 1)],$ 4: $[[[1, 20, 35], 1], ([2, 26, 35], 1),$ $[[7, 40, 35], 1)],$ 6: $[[[2, 26, 39], 1)],$ 9: $[[[16, 34, 18], 1)],$ 13: $[[[10, 25, 35], 1], ([10, 27, 39], -1),$ $[[11, 32, 39], -1], ([15, 33, 31], -1),$ $[[15, 37, 35], -1)],$ 17: $[[[1, 5, 26], 1], ([1, 8, 29], 1),$ $[[19, 35, 26], 1)],$ 21: $[[[18, 31, 39], 1)],$ 22: $[[[1, 5, 40], 1], ([18, 31, 40], 1),$ $[[19, 35, 40], 1)],$ 24: $[[[10, 14, 32], 1], ([10, 16, 34], 1),$ $[[26, 39, 32], 1)],$ 28: $[[[2, 5, 40], 1], ([10, 12, 37], -1),$ $[[25, 35, 40], 1)],$ 30: $[[[33, 15, 12], 1], ([18, 20, 35], 1),$ $[[33, 40, 35], 1)],$ 36: $[[[12, 10, 27], 1], ([25, 26, 39], -1)],$ 38: $[[[12, 10, 29], 1)],$ 41: $[[[5, 1, 23], 1], ([5, 2, 29], 1),$ $[[20, 18, 34], -1)],$ 42: $[[[14, 11, 33], 1], ([32, 31, 40], -1)],$ 43: $[[[14, 10, 29], 1], ([14, 11, 34], 1)],$ 44: $[[[15, 11, 34], 1)]$

## 9 Varieties with singularity

Graph	$\dim(U_o)$	Openings
	8	0: $[[2, 27, 14], 1], ([8, 29, 10], -1),$ $[[8, 38, 12], -1],$ 3: $[[1, 19, 30], 1], ([1, 21, 32], 1),$ $[[7, 37, 30], 1],$ 5: $[[7, 28, 26], 1], ([8, 29, 26], 1),$ 9: $[[11, 30, 19], 1], ([11, 32, 21], 1),$ 13: $[[16, 29, 26], 1],$ 15: $[[11, 30, 37], 1],$ 17: $[[1, 6, 27], 1],$ 22: $[[1, 4, 37], 1], ([18, 30, 37], 1),$ $[[18, 31, 40], 1],$ 23: $[[1, 4, 38], 1],$ 24: $[[10, 14, 32], 1], ([28, 40, 31], -1),$ 35: $[[19, 18, 31], 1], ([37, 33, 31], 1),$ 36: $[[4, 1, 21], 1], ([12, 11, 32], -1),$ $[[19, 18, 32], -1],$ 39: $[[20, 18, 32], 1],$ 42: $[[6, 2, 28], 1],$ 43: $[[6, 2, 29], 1], ([14, 10, 29], 1),$ 44: $[[7, 2, 29], 1], ([7, 4, 38], 1),$ $[[28, 26, 41], -1],$
	8	same but 24: $[[10, 14, 32], 1], ([28, 40, 31], 1),$
	5	0: $[[2, 26, 13], 1], ([7, 44, 16], -1),$ 3: $[[1, 20, 31], 1], ([1, 21, 32], 1),$ $[[7, 42, 32], 1],$ 4: $[[1, 21, 36], 1], ([8, 23, 19], -1),$ $[[2, 27, 36], 1],$ 9: $[[11, 31, 20], 1], ([16, 38, 19], -1),$ 14: $[[10, 25, 36], 1], ([15, 33, 32], -1),$ 17: $[[1, 5, 26], 1], ([1, 6, 27], 1),$ $[[19, 36, 27], 1],$ 22: $[[1, 6, 42], 1], ([1, 8, 44], 1),$ $[[18, 32, 42], 1],$ 24: $[[10, 13, 31], 1],$ 28: $[[2, 6, 42], 1],$ 29: $[[10, 12, 38], 1],$ 30: $[[18, 21, 36], 1],$ 34: $[[33, 15, 16], 1],$ 35: $[[12, 10, 26], 1],$ 37: $[[12, 16, 44], 1],$ 39: $[[5, 1, 21], 1], ([5, 2, 27], 1),$ $[[20, 18, 32], -1],$ 40: $[[13, 11, 33], 1],$ 41: $[[5, 1, 23], 1],$ 43: $[[6, 1, 23], 1], ([6, 7, 44], 1),$ $[[21, 19, 38], -1]$
	5	same but 0: $[[2, 26, 13], 1], ([7, 44, 16], -1)$ 9: $[[11, 31, 20], 1], ([16, 38, 19], 1),$ 14: $[[10, 25, 36], 1], ([15, 33, 32], -1)$
	5	same but 0: $[[2, 26, 13], 1], ([7, 44, 16], 1)$ 9: $[[11, 31, 20], 1], ([16, 38, 19], 1),$ 14: $[[10, 25, 36], 1], ([15, 33, 32], -1)$
	5	other variant on angles 0, 9 and 14.

