

University of Groningen

On approximations, complexity, and applications for copositive programming

Gijben, Luuk

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version

Publisher's PDF, also known as Version of record

Publication date:

2015

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Gijben, L. (2015). *On approximations, complexity, and applications for copositive programming*. [Thesis fully internal (DIV), University of Groningen]. [S.n.].

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Chapter 3

Irreducible elements of the copositive cone ¹

¹Published as [DDGH13a] Peter J.C. Dickinson, Mirjam Dür, Luuk Gijben, and Roland Hildebrand. Irreducible elements of the copositive cone. *Linear Algebra and its Applications*, 439(6):1605-1626, 2013.

In this chapter, we study the structure of \mathcal{COP}^n in relation to the cones \mathcal{S}_+^n and \mathcal{N}^n . We recall from the introduction that if $A \in \mathcal{S}_+^n$ or $A \in \mathcal{N}^n$, then A must be copositive, that is $\mathcal{S}_+^n + \mathcal{N}^n \subseteq \mathcal{COP}^n$. Moreover recall that $\mathcal{S}_+^n + \mathcal{N}^n = \mathcal{COP}^n$ if and only if $n \leq 4$.

From an optimization viewpoint, optimizing over the cone $\mathcal{S}_+^n + \mathcal{N}^n$ is computationally easy as we saw in the Introduction and can be done by standard algorithms like interior point methods, whereas optimizing over \mathcal{COP}^n is hard as we have just seen in the previous chapter. Therefore, the cone \mathcal{COP}^n for $n \geq 5$ is of special interest. Hence, in this chapter we investigate the structure of \mathcal{COP}^n for $n \geq 5$, where we have $\mathcal{COP}^n \neq \mathcal{S}_+^n + \mathcal{N}^n$. Matrices in $\mathcal{COP}^n \setminus (\mathcal{S}_+^n + \mathcal{N}^n)$ have been studied by Johnson and Reams [JR08] who baptized those matrices *exceptional matrices*. As noted before, the Horn matrix (1.10) is in $\mathcal{COP}^n \setminus (\mathcal{S}_+^n + \mathcal{N}^n)$ and therefore is an example of an exceptional matrix.

There are still a number of open problems concerning the cone \mathcal{COP}^n , the characterization of its extreme rays as discussed in the introduction is probably the biggest one. In this chapter we will consider a weaker concept than extremality, namely that of irreducibility with respect to the cone of nonnegative matrices. This property has been utilized and recognized as being more convenient than extremality already in the early work on copositive matrices [Dia62],[HN63],[Bau67]. In particular, it was studied by Baumert [Bau65] who gave a characterization of irreducible matrices. In this chapter, we demonstrate that Baumert's characterization is incorrect and give a correct version of his theorem which establishes a necessary and sufficient condition for a copositive matrix to be irreducible.

For the case of 5×5 copositive matrices we give a complete characterization of all irreducible matrices. We show that those irreducible matrices in \mathcal{COP}^5 which are not positive semidefinite can be parameterized in a semi-trigonometric way. Finally, we prove that every 5×5 copositive matrix which is not the sum of a nonnegative and a semidefinite matrix can be expressed as the sum of a nonnegative and a single irreducible matrix. This last result can be seen as a dual statement to [BAD09, Corollary 2], where it was shown that in the 5×5 case any doubly nonnegative matrix which is not completely positive (such matrices are called "bad matrices" in [BAD09]) can be writ-

ten as the sum of a completely positive matrix and a single "extremely bad" matrix (i.e., a matrix which is extremal for the doubly nonnegative cone, but not completely positive).

3.1 Notation

During this chapter we let \mathbf{e}_i be the unit vector with the i th element equal to one and all other elements equal to 0. For simplicity we shall also denote $\mathbf{e}_{ij} = \mathbf{e}_i + \mathbf{e}_j$ for $i \neq j$.

For a vector $\mathbf{u} \in \mathbb{R}_+^n$ we define its support as

$$\text{supp}(\mathbf{u}) := \{i \in \{1, \dots, n\} \mid u_i > 0\}.$$

For a set $\mathcal{M} \subseteq \mathbb{R}_+^n$ we shall define its support as

$$\text{supp}(\mathcal{M}) := \{\text{supp}(\mathbf{u}) \mid \mathbf{u} \in \mathcal{M}\}.$$

For a subset $\mathcal{I} \subseteq \{1, \dots, n\}$ we denote by $A_{\mathcal{I}}$ the principal submatrix of A whose elements have row and column indices in \mathcal{I} , i.e. $A_{\mathcal{I}} := (a_{ij})_{i,j \in \mathcal{I}}$. Similarly for a vector $\mathbf{v} \in \mathbb{R}^n$ we denote the subvector $\mathbf{u}_{\mathcal{I}} := (u_i)_{i \in \mathcal{I}}$.

For $i, j = 1, \dots, n$, we denote the following generators of the extreme rays of the nonnegative cone \mathcal{N}^n by

$$E_{\{ij\}} := \begin{cases} \mathbf{e}_i \mathbf{e}_i^{\top} & \text{if } i = j \\ \mathbf{e}_i \mathbf{e}_j^{\top} + \mathbf{e}_j \mathbf{e}_i^{\top} & \text{otherwise.} \end{cases}$$

This notation is not to be confused with E , the matrix of all ones, or the matrices E^{ij} that were defined before, and who are in a sense the non-symmetric versions of the matrices $E_{\{ij\}}$. We call a nonzero vector $\mathbf{u} \in \mathbb{R}_+^n$ a *zero* of a copositive matrix $A \in \mathcal{COP}^n$ if $\mathbf{u}^{\top} A \mathbf{u} = 0$. We denote the set of zeros of A by

$$\mathcal{V}^A := \{\mathbf{u} \in \mathbb{R}_+^n \setminus \{\mathbf{0}\} \mid \mathbf{u}^{\top} A \mathbf{u} = 0\}.$$

This notation is similar to that used by Dickinson in [Dic10], except for the fact that we will exclude the vector $\mathbf{0}$ from the set.

Let $\text{Aut}(\mathbb{R}_+^n)$ be the automorphism group of the nonnegative orthant. It is generated by all $n \times n$ permutation matrices and by all $n \times n$ diagonal matrices with strictly positive diagonal elements. This group generates a group \mathcal{G}_n of automorphisms of \mathcal{COP}^n by $A \mapsto AXA^{\top}$, $A \in \text{Aut}(\mathbb{R}_+^n)$. Whenever we speak of orbits of elements in \mathcal{COP}^n , we mean orbits with respect to the action of \mathcal{G}_n .

Definition 3.1. For a matrix $A \in \mathcal{COP}^n$ and a set \mathcal{M} contained in the space of symmetric matrices, we say that A is \mathcal{M} -irreducible if there do not exist $\gamma > 0$ and $M \in \mathcal{M} \setminus \{0\}$ such that $A - \gamma M \in \mathcal{COP}^n$.

Note that this definition differs from the concept of an irreducible matrix that is normally used in matrix theory. We will synonymously use the expressions of being \mathcal{M} -irreducible and being irreducible with respect to \mathcal{M} . For simplicity we speak about irreducibility with respect to M when $\mathcal{M} = \{M\}$. During this chapter, we shall be concerned with the cases

$$\mathcal{M} = \mathcal{N}^n, \quad \mathcal{M} = \tilde{\mathcal{N}}^n, \quad \text{and} \quad \mathcal{M} = \{E_{\{ij\}}\}.$$

where $\tilde{\mathcal{N}}^n := \{N \in \mathcal{N}^n \mid \text{diag}(N) = \mathbf{0}\}$. The $A^*(n; 0)$ -property defined in [Dia62, p.17] or, equivalently, the $A^*(n)$ -property² defined in [Bau66, Def. 2.1] are then equivalent to being irreducible with respect to \mathcal{N}^n .

It is easy to see that an irreducible matrix necessarily is in the boundary of \mathcal{COP}^n . Also note that if a nonzero matrix A is on an extreme ray of \mathcal{COP}^n , then A must be \mathcal{N}^n -irreducible: indeed, assume the contrary. Then there exist $\gamma > 0$ and $0 \neq N \in \mathcal{N}^n$ such that $A - \gamma N =: B \in \mathcal{COP}^n$. But then $A = B + \gamma N$, contradicting extremality.

Observe that being $\tilde{\mathcal{N}}^n$ -irreducible is a weaker condition than being \mathcal{N}^n -irreducible. It is also trivial to see that $A \in \mathcal{COP}^n$ is irreducible with respect to \mathcal{N}^n if and only if it is irreducible with respect to $E_{\{ij\}}$ for all $i, j = 1, \dots, n$, whilst A is irreducible with respect to $\tilde{\mathcal{N}}^n$ if and only if it is irreducible with respect to $E_{\{ij\}}$ for all $i \neq j$.

3.2 Irreducible copositive matrices

In this section we shall show that the following theorem from Baumert's thesis [Bau65] about irreducibility with respect to $E_{\{ij\}}$ is incorrect, and we shall give the corrected version of this theorem.

Assertion 3.2 (Incorrect Theorem 3.3 of [Bau65]). *For $i, j = 1, \dots, n$ we have that a matrix $A \in \mathcal{COP}^n$ is irreducible with respect to $E_{\{ij\}}$ if and only if there exists a vector $\mathbf{u} \in \mathcal{V}^A$ such that $u_i u_j > 0$.*

It is trivial to see that the reverse implication holds, as for such a \mathbf{u} and any $\gamma > 0$ we have that $\mathbf{u}^\top (A - \gamma E_{\{ij\}}) \mathbf{u} = -2\gamma u_i u_j < 0$. However the following

²This notation is also used in [Dia62], but without definition.

matrix is a counterexample to the forward implication:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix} \quad (3.1)$$

In order to show this we need the following lemma.

Lemma 3.3. *Let $A \in \mathcal{S}_+^n$. Then $\mathbf{u} \in \mathbb{R}^n$ is a zero of A , that is $\mathbf{u}^\top A \mathbf{u} = 0$, if and only if $A \mathbf{u} = \mathbf{0}$.*

Proof. Let $A \in \mathcal{S}_+^n$ and suppose that $\mathbf{u} \in \mathbb{R}^n$ is such that $\mathbf{u}^\top A \mathbf{u} = 0$. Then because $A \in \mathcal{S}_+^n$ we can write $A = BB^\top$ and hence

$$0 = \mathbf{u}^\top A \mathbf{u} = \mathbf{u}^\top B B^\top \mathbf{u} = (B^\top \mathbf{u})^\top (B^\top \mathbf{u}) = \mathbf{y}^\top \mathbf{y} = \sum_{i=1}^n (y_i)^2.$$

This can obviously only happen if $y_i = 0$ for all $i = 1, \dots, n$, which means that we have $A \mathbf{u} = B(B^\top \mathbf{u}) = \mathbf{0}$.

On the other hand if $A \mathbf{u} = \mathbf{0}$ then obviously $\mathbf{u}^\top A \mathbf{u} = 0$. □

Now because A , as defined by (3.1), is positive semidefinite and because we have that $\mathbf{x}^\top A \mathbf{x} = 0$ if and only if $A \mathbf{x} = \mathbf{0}$ we get that $\mathcal{V}^A = \{\lambda \mathbf{e}_{23} \mid \lambda > 0\}$. Therefore, according to Baumert's theorem, A should be irreducible *only* with respect to $E_{\{23\}}$, and hence A should *not* be irreducible with respect to, say, $E_{\{12\}}$. In other words, there should exist a $\gamma > 0$ such that $A - \gamma E_{\{12\}}$ is copositive. However, for any $\gamma > 0$ we have

$$\begin{pmatrix} \gamma \\ 1 \\ 1 \end{pmatrix}^\top \begin{pmatrix} 1 & -\gamma & 0 \\ -\gamma & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} \gamma \\ 1 \\ 1 \end{pmatrix} = -\gamma^2 < 0,$$

which demonstrates that A is also irreducible with respect to $E_{\{12\}}$, contradicting Baumert's theorem.

As [Bau65, Theorem 3.3] is incorrect³, also other results from Baumert's

³The proof of Theorem 3.3 of [Bau65] contains two errors, each of which leads to counterexamples. One error is the omission of the multiples of $E_{\{11\}}$ in the classification making up the inductive base on page 12 of Baumert's thesis [Bau65]. (Note that for the 2×2 case, the matrix $E_{\{11\}}$ also provides a counterexample to Baumert's assertion.) The other error, being located in the induction step for case 3 on page 14, is more subtle. Generally, in order for an induction step to be applicable, the problem in question has to be reduced to an instance of the same problem of strictly smaller size. In the proof this is to be ensured by the fact that the copositive form Q_2 depends on a strictly smaller number of variables than the original form Q , in particular, because Q_2 does no more depend on the variable x_2 . However, since irreducibility with respect to $E_{\{12\}}$ is studied, dependence on x_2 has nevertheless to be formally included. Therefore, the induction step is applicable only if either the support of the zero \mathbf{u} is strictly bigger than $\{2\}$, or the support of $Q\mathbf{u}$ is nonempty. Both conditions may simultaneously fail to be satisfied, however.

thesis [Bau65] which are proved using this result must be treated with care. Fortunately this error has not entered into Baumert's papers [Bau66, Bau67], which as far as we can tell are correct. In our paper we do use results from Baumert's papers, and to make sure that this error could not have had an effect, we made sure that they were correct from first principles.

For easy reference in the remainder of the paper, we reference the property used in Baumert's incorrect theorem as follows:

Property 3.4. *For each pair i, j of indices such that $i \neq j$, there exists a zero \mathbf{u} of A such that $u_i u_j > 0$.*

Our next aim is to present a corrected version of this theorem. Before doing so, however, we first discuss a couple of properties related to the set of zeros.

Lemma 3.5 (p. 200 of [Bau66]). *Let $A \in \mathcal{COP}^n$ and $\mathbf{u} \in \mathcal{V}^A$. Then $A\mathbf{u} \geq \mathbf{0}$.*

Lemma 3.6. *Let $A \in \mathcal{COP}^n$ and $\mathbf{u} \in \mathcal{V}^A$. Then the principal submatrix $A_{\text{supp}(\mathbf{u})}$ is positive semidefinite.*

Proof. Clearly, \mathbf{u} is a zero of A if and only if $\mathbf{u}_{\text{supp}(\mathbf{u})}$ is a zero of $A_{\text{supp}(\mathbf{u})}$. Moreover, $\mathbf{u}_{\text{supp}(\mathbf{u})} > \mathbf{0}$. Therefore, by [Dia62, Lemma 1], we have that

$$(\mathbf{u}_{\text{supp}(\mathbf{u})})^\top A_{\text{supp}(\mathbf{u})} (\mathbf{u}_{\text{supp}(\mathbf{u})}) = \mathbf{0}$$

implies that $A_{\text{supp}(\mathbf{u})}$ is positive semidefinite. □

Lemma 3.7. *Let $A \in \mathcal{COP}^n$ and $\mathbf{u}, \mathbf{v} \in \mathcal{V}^A$ such that $\text{supp}(\mathbf{u}) \subseteq \text{supp}(\mathbf{v})$. Then we have that $(A\mathbf{u})_i = 0$ for all $i \in \text{supp}(\mathbf{v})$.*

Proof. This comes trivially from the previous lemma and recalling that for arbitrary $B \in \mathcal{S}_+^m$ and $\mathbf{v} \in \mathbb{R}^m$ we have that $\mathbf{v}^\top B \mathbf{v} = 0$ if and only if $B\mathbf{v} = \mathbf{0}$. □

Note that applying the previous lemma for $\mathbf{u} = \mathbf{v}$ gives us that $A \in \mathcal{COP}^n$ and $\mathbf{u} \in \mathcal{V}^A$ imply that $(A\mathbf{u})_i = 0$ for all $i \in \text{supp}(\mathbf{u})$.

We now present the main theorem of this section, which is the corrected version of Baumert's theorem.

Theorem 3.8. *Let $A \in \mathcal{COP}^n$, $n \geq 2$, and let $1 \leq i, j \leq n$. Then the following conditions are equivalent.*

- (i) *A is irreducible with respect to $E_{\{ij\}}$,*
- (ii) *there exists $\mathbf{u} \in \mathcal{V}^A$ such that $(A\mathbf{u})_i = (A\mathbf{u})_j = 0$ and $u_i + u_j > 0$.*

Proof. The special case when $i = j$ is proven in [Bau66, Theorem 3.4], so from now on we shall consider $i \neq j$. For $\varepsilon > 0$, we will abbreviate $A_\varepsilon := A - \varepsilon E_{\{ij\}}$.

We first show (ii) \Rightarrow (i). Assume that there exists such a $\mathbf{u} \in \mathcal{V}^A$. Fix $\varepsilon > 0$ and let $\delta > 0$. Then $\mathbf{u} + \delta \mathbf{e}_{ij} \geq 0$ and

$$\begin{aligned} (\mathbf{u} + \delta \mathbf{e}_{ij})^\top A_\varepsilon (\mathbf{u} + \delta \mathbf{e}_{ij}) &= \mathbf{u}^\top A \mathbf{u} + 2\delta \mathbf{e}_{ij}^\top A \mathbf{u} + \delta^2 (a_{ii} + 2a_{ij} + a_{jj}) - 2\varepsilon (u_i + \delta)(u_j + \delta) \\ &= -2\varepsilon u_i u_j - 2\varepsilon \delta (u_i + u_j) + \mathcal{O}(\delta^2). \end{aligned}$$

Since $u_i u_j \geq 0$ and $u_i + u_j > 0$, this term is negative for $\delta > 0$ small enough. Hence A_ε is not copositive and A satisfies condition (i).

Let us now show (i) \Rightarrow (ii) by induction over n . For $n = 2$, it can be seen that copositive matrices satisfying condition (i) are of the form

$$\begin{pmatrix} a^2 & -ab \\ -ab & b^2 \end{pmatrix} \quad \text{with } a, b \geq 0.$$

If $a = b = 0$, then any $\mathbf{u} \in \mathbb{R}_+^n \setminus \{\mathbf{0}\}$ satisfies condition (ii). Alternatively, if $a + b > 0$, then the zero $\mathbf{u} = (b, a)^\top$ satisfies condition (ii).

Now assume that the assertion holds for $\hat{n} < n$, and let $A \in \mathcal{COP}^n$ satisfy condition (i). For every $\varepsilon > 0$, consider the optimization problem

$$\min \left\{ \frac{1}{2} \mathbf{v}^\top A_\varepsilon \mathbf{v} \mid \mathbf{v} \in \mathbb{R}_+^n, \mathbf{e}^\top \mathbf{v} = 1 \right\}. \quad (3.2)$$

By condition (i) the optimal value of this problem is negative, and it is attained by compactness of the feasible set. Let \mathbf{v} be a minimizer of the problem. Having only linear constraints, the problem fulfills a constraint qualification, and therefore it follows from the Karush-Kuhn-Tucker optimality conditions that there exist Lagrange multipliers $\boldsymbol{\lambda} \in \mathbb{R}_+^n$ and $\mu \in \mathbb{R}$ such that $\mathbf{v}^\top \boldsymbol{\lambda} = 0$ and $A_\varepsilon \mathbf{v} - \boldsymbol{\lambda} + \mu \mathbf{e} = 0$, or equivalently,

$$A_\varepsilon \mathbf{v} = \boldsymbol{\lambda} - \mu \mathbf{e}. \quad (3.3)$$

Multiplying with \mathbf{v}^\top and observing $\mathbf{v}^\top \boldsymbol{\lambda} = 0$ and $\mathbf{v}^\top \mathbf{e} = 1$, we obtain $-\mu = \mathbf{v}^\top A_\varepsilon \mathbf{v} < 0$. We also have $\mathbf{v}^\top A \mathbf{v} - 2\varepsilon v_i v_j = \mathbf{v}^\top A_\varepsilon \mathbf{v} < 0$, which by $\mathbf{v}^\top A \mathbf{v} \geq 0$ yields $v_i > 0, v_j > 0$. Therefore $\lambda_i = \lambda_j = 0$, and

$$(A_\varepsilon \mathbf{v})_i = (A_\varepsilon \mathbf{v})_j = -\mu < 0. \quad (3.4)$$

Let now $\varepsilon_k \rightarrow 0$, let $\mathbf{v}^k \in \mathbb{R}_+^n$ be a minimizer of problem (3.2) for $\varepsilon = \varepsilon_k$, and let $\boldsymbol{\lambda}^k = (\lambda_1^k, \dots, \lambda_n^k)$, μ^k be the corresponding Lagrange multipliers. By possibly choosing a subsequence, we can assume w.l.o.g. that $\mathbf{v}^k \rightarrow \mathbf{v}^* \in \mathbb{R}_+^n \setminus \{\mathbf{0}\}$. Then $0 \geq \lim_{k \rightarrow \infty} \mathbf{v}^{k \top} A_{\varepsilon_k} \mathbf{v}^k = \mathbf{v}^{* \top} A \mathbf{v}^* \geq 0$, and hence by Lemma 3.5

$A\mathbf{v}^* \geq \mathbf{0}$. Since $\lim_{k \rightarrow \infty} A_{\varepsilon_k} \mathbf{v}^k = A\mathbf{v}^* \geq \mathbf{0}$, we get from (3.4) that $(A\mathbf{v}^*)_i = (A\mathbf{v}^*)_j = 0$. If $v_i^* + v_j^* > 0$, then \mathbf{v}^* verifies condition (ii). Hence assume that $v_i^* = v_j^* = 0$ and consider two cases:

Case 1: Suppose there exists an index l such that $(A\mathbf{v}^*)_l > 0$. Then $i \neq l \neq j$. From (3.3) we obtain $(A_{\varepsilon_k} \mathbf{v}^k)_l = \lambda_l^k - \mu^k < \lambda_l^k$ for all k . By $\lim_{k \rightarrow \infty} (A_{\varepsilon_k} \mathbf{v}^k)_l = (A\mathbf{v}^*)_l > 0$ we must have $\lambda_l^k > 0$ for k large enough, and hence $(\boldsymbol{\lambda}^k)^\top \mathbf{v}^k = 0$ implies $\mathbf{v}_l^k = 0$ for those k . This implies that

$$0 > (\mathbf{v}^k)^\top (A - \varepsilon_k E_{\{ij\}}) \mathbf{v}^k = (\hat{\mathbf{v}}^k)^\top (\hat{A} - \varepsilon_k \hat{E}_{\{ij\}}) \hat{\mathbf{v}}^k$$

where \hat{A} (resp. $\hat{E}_{\{ij\}}$) are the principal submatrices of A (resp. $E_{\{ij\}}$) obtained by crossing out row and column l , and $\hat{\mathbf{v}}^k$ is obtained from \mathbf{v}^k by crossing out row l . This means that \hat{A} is irreducible with respect to $\hat{E}_{\{ij\}}$. By the induction hypothesis, there exists a zero $\hat{\mathbf{u}}$ of \hat{A} satisfying condition (ii). The sought zero \mathbf{u} of A can then be obtained by inserting a '0' in $\hat{\mathbf{u}}$ at position l , which concludes the proof for this case.

Case 2: Suppose now that $A\mathbf{v}^* = \mathbf{0}$. Let $\mathcal{I} = \text{supp}(\mathbf{v}^*)$ and let $\mathcal{J} = \{1, \dots, n\} \setminus \mathcal{I}$. Note that $i, j \in \mathcal{J}$ and that $|\mathcal{J}| < n$. By [Bau66, Lemma 3.1] we can represent A as $A = P + C$, where P is positive semidefinite, the principal submatrix $P_{\mathcal{J}}$ has the same rank as P , and C is a copositive matrix whose principal submatrix $C_{\mathcal{J}}$ contains all its nonzero elements. The property $\mathbf{v}^{*\top} A\mathbf{v}^* = 0$ implies $P\mathbf{v}^* = \mathbf{0}$ and $\mathbf{v}^{*\top} C\mathbf{v}^* = 0$. Moreover, $C\mathbf{v}^* = \mathbf{0}$ by construction. The matrix C is irreducible with respect to $E_{\{ij\}}$, and hence $C_{\mathcal{J}}$ is irreducible with respect to $(E_{\{ij\}})_{\mathcal{J}}$. By the induction hypothesis on $C_{\mathcal{J}}$ there exists a zero with the sought properties which we can augment to obtain a zero \mathbf{u} of C with $(C\mathbf{u})_i = (C\mathbf{u})_j = 0$, $u_i + u_j > 0$, and $u_l = 0$ for all $l \in \mathcal{I}$. By the rank property of P there exists a vector $\tilde{\mathbf{u}}$ such that $\tilde{u}_l = u_l$ for all $l \in \mathcal{J}$ and $P\tilde{\mathbf{u}} = \mathbf{0}$. Since $\tilde{u}_l \geq 0$ for all $l \in \mathcal{J}$, there exists $\alpha \geq 0$ such that $\mathbf{w} := \tilde{\mathbf{u}} + \alpha \mathbf{v}^* \geq \mathbf{0}$. Then we have $P\mathbf{w} = \mathbf{0}$ and $\mathbf{w}^\top A\mathbf{w} = \mathbf{w}^\top C\mathbf{w} = \tilde{\mathbf{u}}^\top C\tilde{\mathbf{u}} = \mathbf{u}^\top C\mathbf{u} = 0$ and $A\mathbf{w} = C\mathbf{w} = C\tilde{\mathbf{u}} = C\mathbf{u}$. It follows that $(A\mathbf{w})_i = (A\mathbf{w})_j = 0$, and moreover $w_i + w_j = u_i + u_j > 0$. Thus A satisfies condition (ii), which completes the proof of the theorem. \square

Related to this theorem we define the following.

Definition 3.9. Let $A \in \mathcal{COP}^n$ be irreducible with respect to $E_{\{ij\}}$. If $\mathbf{u} \in \mathcal{V}^A$ satisfies condition (ii) in Theorem 3.8, then we say that irreducibility with respect to $E_{\{ij\}}$ is *associated to \mathbf{u}* , or for short, $E_{\{ij\}}$ is *associated to \mathbf{u}* .

As a consequence of Theorem 3.8, a matrix $A \in \mathcal{COP}^n$ is irreducible with respect to $\tilde{\mathcal{N}}^n$ if and only if it satisfies the following property.

Property 3.10. *For each index pair (i, j) with $i < j$, there exists $\mathbf{u} \in \mathcal{V}^A$ such that at least one of the following holds:*

- $u_i u_j > 0$,
- $u_i > 0$ and $u_j = (\mathbf{A}\mathbf{u})_j = 0$,
- $u_j > 0$ and $u_i = (\mathbf{A}\mathbf{u})_i = 0$.

Another consequence of Theorem 3.8 is that a matrix $A \in \mathcal{COP}^n$ is irreducible with respect to \mathcal{N}^n if and only if it satisfies Property 3.10 and for all $i = 1, \dots, n$ there exists $\mathbf{u} \in \mathcal{V}^A$ with $u_i > 0$.

Note that Property 3.10 is weaker than Property 3.4. In the next section we consider explicit examples of matrices $A \in \mathcal{COP}^5$ which satisfy Property 3.10, but not Property 3.4.

3.3 *S*-matrices

In this section we consider matrices of the form

$$S(\boldsymbol{\theta}) = \begin{pmatrix} 1 & -\cos \theta_1 & \cos(\theta_1 + \theta_2) & \cos(\theta_4 + \theta_5) & -\cos \theta_5 \\ -\cos \theta_1 & 1 & -\cos \theta_2 & \cos(\theta_2 + \theta_3) & \cos(\theta_5 + \theta_1) \\ \cos(\theta_1 + \theta_2) & -\cos \theta_2 & 1 & -\cos \theta_3 & \cos(\theta_3 + \theta_4) \\ \cos(\theta_4 + \theta_5) & \cos(\theta_2 + \theta_3) & -\cos \theta_3 & 1 & -\cos \theta_4 \\ -\cos \theta_5 & \cos(\theta_5 + \theta_1) & \cos(\theta_3 + \theta_4) & -\cos \theta_4 & 1 \end{pmatrix} \quad (3.5)$$

with $\boldsymbol{\theta} \in \mathbb{R}_+^5$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$. Note that the Horn matrix H from (1.10) is of this form with $\boldsymbol{\theta} = \mathbf{0}$. It is easy to verify that H satisfies Property 3.4. The Horn matrix has been shown to be extremal for the cone of copositive matrices \mathcal{COP}^5 , see [HN63].

The matrices $S(\boldsymbol{\theta})$ are transformed versions of the matrices $T(\boldsymbol{\varphi})$ that were introduced by Hildebrand in [Hil12] by making a trivial substitution. Observe, however, that we study $S(\boldsymbol{\theta})$ with $\boldsymbol{\theta}$ in a different range: While Hildebrand [Hil12] showed that an $S(\boldsymbol{\theta})$ with $\boldsymbol{\theta} \in \mathbb{R}_{++}^5$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$ is extremal for \mathcal{COP}^5 , we specifically consider in this section $S(\boldsymbol{\theta})$ with $\boldsymbol{\theta} \in \mathbb{R}_+^5 \setminus (\mathbb{R}_{++}^5 \cup \{\mathbf{0}\})$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$. We show that these matrices provide further counterexamples to Baumert's theorem. Moreover these matrices will also be of use later in this chapter.

Theorem 3.11. *Let $\boldsymbol{\theta} \in \mathbb{R}_+^5 \setminus (\mathbb{R}_{++}^5 \cup \{\mathbf{0}\})$ such that $\mathbf{e}^\top \boldsymbol{\theta} < \pi$. Then the matrix $S(\boldsymbol{\theta})$ is in \mathcal{COP}^5 , not extremal, not positive semidefinite, irreducible with respect to \mathcal{N}^5 and satisfies Property 3.10, but not Property 3.4.*

Proof. Without loss of generality we can always cycle the indices so we can assume that $\theta_1 = 0$. It is then easy to verify that

$$S(\boldsymbol{\theta}) = \mathbf{a}\mathbf{a}^\top + \text{Diag}(\mathbf{d})H\text{Diag}(\mathbf{d})$$

where H is the Horn matrix (1.10),

$$\mathbf{a} = \begin{pmatrix} -\sin(\frac{1}{2}(\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ \sin(\frac{1}{2}(\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ -\sin(\frac{1}{2}(-\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ \sin(\frac{1}{2}(-\theta_2 - \theta_3 + \theta_4 + \theta_5)) \\ -\sin(\frac{1}{2}(-\theta_2 - \theta_3 - \theta_4 + \theta_5)) \end{pmatrix}, \quad \text{and} \quad \mathbf{d} = \begin{pmatrix} \cos(\frac{1}{2}(\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ \cos(\frac{1}{2}(\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ \cos(\frac{1}{2}(-\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ \cos(\frac{1}{2}(-\theta_2 - \theta_3 + \theta_4 + \theta_5)) \\ \cos(\frac{1}{2}(-\theta_2 - \theta_3 - \theta_4 + \theta_5)) \end{pmatrix}.$$

We have $\mathbf{d} > 0$ from which we see that $S(\boldsymbol{\theta})$ is copositive. We also have that $\mathbf{a} \neq \mathbf{0}$ from which we see that $S(\boldsymbol{\theta})$ is not extremal. For the set of zeros of $S(\boldsymbol{\theta})$ it can be seen that

$$\begin{aligned} \mathcal{V}^{S(\boldsymbol{\theta})} &= \text{Diag}(\mathbf{d})^{-1} \mathcal{V}^{\text{Diag}(\mathbf{d})^{-1} S(\boldsymbol{\theta}) \text{Diag}(\mathbf{d})^{-1}} \\ &= \text{Diag}(\mathbf{d})^{-1} \left(\mathcal{V}^{(\text{Diag}(\mathbf{d})^{-1} \mathbf{a})(\text{Diag}(\mathbf{d})^{-1} \mathbf{a})^\top} \cap \mathcal{V}^H \right) \\ &= \text{Diag}(\mathbf{d})^{-1} \left\{ \mathbf{x} \in \mathcal{V}^H \mid \mathbf{x}^\top (\text{Diag}(\mathbf{d})^{-1} \mathbf{a}) = 0 \right\}, \end{aligned}$$

where we observe that

$$\mathcal{V}^H = \bigcup_{\substack{\text{cyclic} \\ \text{permutations}}} \text{cone} \left\{ \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right\} \setminus \{\mathbf{0}\},$$

and

$$\text{Diag}(\mathbf{d})^{-1} \mathbf{a} = \begin{pmatrix} -\tan(\frac{1}{2}(\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ \tan(\frac{1}{2}(\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ -\tan(\frac{1}{2}(-\theta_2 + \theta_3 + \theta_4 + \theta_5)) \\ \tan(\frac{1}{2}(-\theta_2 - \theta_3 + \theta_4 + \theta_5)) \\ -\tan(\frac{1}{2}(-\theta_2 - \theta_3 - \theta_4 + \theta_5)) \end{pmatrix}.$$

If $\mathbf{u} \in \mathcal{V}^{S(\boldsymbol{\theta})}$ then we have that $S(\boldsymbol{\theta})\mathbf{u} = \text{Diag}(\mathbf{d})H\text{Diag}(\mathbf{d})\mathbf{u}$. From this we observe that:

- If $\mathbf{u} \in \mathcal{V}^{S(\boldsymbol{\theta})}$ such that $\text{supp}(\mathbf{u}) = \{1, 2\}$, then $\text{supp}(S(\boldsymbol{\theta})\mathbf{u}) = \{4\}$.
- If $\mathbf{u} \in \mathcal{V}^{S(\boldsymbol{\theta})}$ such that $\text{supp}(\mathbf{u}) = \{1, 2, 3\}$, then $\text{supp}(S(\boldsymbol{\theta})\mathbf{u}) = \{4, 5\}$.

These results apply similarly after cyclic permutations.

For $i, j \in \{1, \dots, 5\}$ we now say that (i, j) has Property I or Property II if and only if the following respective conditions hold:

I. There exists $\mathbf{u} \in \mathcal{V}^{S(\boldsymbol{\theta})}$ such that $u_i u_j > 0$.

II. There exists $\mathbf{u} \in \mathcal{V}^{S(\boldsymbol{\theta})}$ such that $u_i > 0 = u_j$ and $(S(\boldsymbol{\theta})\mathbf{u})_j = 0$.

We then have that $S(\boldsymbol{\theta})$ satisfies Property 3.4 if and only if for all $i, j = 1, \dots, 5$ we have that (i, j) satisfies Property I, and $S(\boldsymbol{\theta})$ satisfies Property 3.10 if and only if for all $i, j = 1, \dots, 5$, $i < j$ at least one of (i, j) or (j, i) satisfies at least one of properties I or II.

Without loss of generality (by considering cyclic permutations) we now have 6 cases to consider. For each case, by looking at the structure of $\text{Diag}(\mathbf{d})^{-1}\mathbf{a}$ and \mathcal{V}^H it is a trivial but somewhat tedious task to find the support of the set of zeros. From this we can use the results above to check for each (i, j) if Property I or II holds. In each case we will name the case, give the support of the set of zeros and give a table showing for each (i, j) if Property I or II holds.

1. $\theta_1 = \theta_2 = \theta_3 = \theta_4 = 0$ and $0 < \theta_5 < \pi$: We have

$$\text{supp} \left(\mathcal{V}^{S(\boldsymbol{\theta})} \right) = \left\{ \{1, 2\}, \{2, 3\}, \{3, 4\}, \{4, 5\}, \{1, 2, 3\}, \{2, 3, 4\}, \{3, 4, 5\} \right\}$$

and

$j \setminus i$	1	2	3	4	5
1	I	I	I,II		II
2	I,II	I	I,II	I,II	II
3	I,II	I,II	I	I,II	I,II
4	II	I,II	I,II	I	I,II
5	II		I,II	I	I

2. $\theta_1 = \theta_2 = \theta_3 = 0$ and $0 < \theta_4, \theta_5$ and $\theta_4 + \theta_5 < \pi$: We have

$$\text{supp} \left(\mathcal{V}^{S(\boldsymbol{\theta})} \right) = \left\{ \{1, 2\}, \{2, 3\}, \{3, 4\}, \{1, 2, 3\}, \{2, 3, 4\}, \{1, 4, 5\} \right\}$$

and

$j \setminus i$	1	2	3	4	5
1	I	I	I,II	I	I,II
2	I,II	I	I,II	I,II	II
3	I,II	I,II	I	I,II	II
4	I	I,II	I	I	I,II
5	I			I	I

3. $\theta_1 = \theta_2 = \theta_4 = 0$ and $0 < \theta_3, \theta_5$ and $\theta_3 + \theta_5 < \pi$: We have

$$\text{supp} \left(\mathcal{V}^{S(\theta)} \right) = \left\{ \{1, 2\}, \{2, 3\}, \{4, 5\}, \{1, 2, 3\} \right\}$$

and

$j \setminus i$	1	2	3	4	5
1	I	I	I,II		II
2	I,II	I	I,II	II	II
3	I,II	I	I	II	
4	II		II	I	I
5	II		II	I	I

4. $\theta_1 = \theta_2 = 0$ and $0 < \theta_3, \theta_4, \theta_5$ and $\theta_3 + \theta_4 + \theta_5 < \pi$: We have

$$\text{supp} \left(\mathcal{V}^{S(\theta)} \right) = \left\{ \{1, 2\}, \{2, 3\}, \{1, 2, 3\}, \{2, 3, 4\}, \{1, 4, 5\} \right\}$$

and

$j \setminus i$	1	2	3	4	5
1	I	I	I,II	I	I,II
2	I,II	I	I,II	II	II
3	I,II	I	I	I,II	I
4	I		I	I	I
5	I		I	I	I

5. $\theta_1 = \theta_3 = 0$ and $0 < \theta_2, \theta_4, \theta_5$ and $\theta_2 + \theta_4 + \theta_5 < \pi$: We have

$$\text{supp} \left(\mathcal{V}^{S(\theta)} \right) = \left\{ \{1, 2\}, \{3, 4\}, \{1, 4, 5\} \right\}$$

and

$j \setminus i$	1	2	3	4	5
1	I	I	II	I	I,II
2	I	I	II		II
3		II	I	I	II
4	I	II	I	I	I,II
5	I			I	I

6. $\theta_1 = 0$ and $0 < \theta_2, \theta_3, \theta_4, \theta_5$ and $\theta_2 + \theta_3 + \theta_4 + \theta_5 < \pi$: We have

$$\text{supp} \left(\mathcal{V}^{S(\theta)} \right) = \left\{ \{1, 2\}, \{2, 3, 4\}, \{3, 4, 5\}, \{1, 4, 5\} \right\}$$

and

$j \setminus i$	1	2	3	4	5
1	I	I	II	I	I,II
2	I	I	I,II	I	II
3		I	I	I	I
4	I	I	I	I	I
5	I		I	I	I

From analyzing these results we see that in each case the matrix $S(\boldsymbol{\theta})$ satisfies Property 3.10 but not Property 3.4. Since (i, i) always has Property I it follows that $S(\boldsymbol{\theta})$ is irreducible with respect to \mathcal{N}^5 .

Now let (i, j) have neither Property I nor Property II. From the tables above one can see that such a pair always exists. Let $\mathbf{u} \in \mathcal{V}^{S(\boldsymbol{\theta})}$ be such that $u_i > 0$. If now $S(\boldsymbol{\theta}) \in \mathcal{S}_+^5$, then $S(\boldsymbol{\theta})\mathbf{u} = \mathbf{0}$. Therefore, if $u_j > 0$, then (i, j) has Property I, and if $u_j = 0$, then (i, j) has Property II. Thus we obtain a contradiction, which proves that $S(\boldsymbol{\theta})$ is not positive semidefinite. This completes the proof. \square

3.4 Auxiliary results

We next want to study the form of irreducible matrices. We start with two trivial, but important, lemmas.

Lemma 3.12. *For $n \geq 2$, let $A \in \mathcal{COP}^n$ and $i \in \{1, \dots, n\}$ such that $A_{ii} = 0$. Then A is irreducible with respect to $\tilde{\mathcal{N}}^n$ if and only if $a_{ij} = 0$ for all $j = 1, \dots, n$, and $A_{\{1, \dots, n\} \setminus \{i\}}$ is irreducible with respect to $\tilde{\mathcal{N}}^{n-1}$.*

Proof. This is trivial to see after recalling that every principle submatrix of a copositive matrix must be copositive. \square

Lemma 3.13. *Let $A \in \mathcal{S}_+^n + \mathcal{N}^n$ be irreducible with respect to $\tilde{\mathcal{N}}^n$. Then $A \in \mathcal{S}_+^n$.*

Proof. This is trivial to see from

$$\mathcal{N}^n \setminus \tilde{\mathcal{N}}^n = \{\text{Diag}(\mathbf{d}) \mid \mathbf{d} \in \mathbb{R}_+^n\} \setminus \{\mathbf{0}\} \subset \mathcal{S}_+^n$$

and $\mathcal{S}_+^n + \mathcal{N}^n \subseteq \mathcal{COP}^n$. \square

Note again that for $n \leq 4$ we have $\mathcal{S}_+^n + \mathcal{N}^n = \mathcal{COP}^n$, so in these cases all of the matrices which are irreducible with respect to $\tilde{\mathcal{N}}^n$ must be positive semidefinite. We will however now consider order 2 and order 3 copositive matrices more specifically. Due to Lemma 3.12 we may limit ourselves to

cases when all the on-diagonal elements are strictly positive. By considering scaling with a diagonal matrix with on-diagonal elements strictly positive, we can in fact limit ourselves to the case where all the on-diagonal elements are equal to one.

Lemma 3.14. *Let $A \in \mathcal{COP}^2$ be such that $\text{diag}(A) = \mathbf{e}$. Then we have that $\mathcal{V}^A \subseteq \{\lambda \mathbf{e}_{12} \mid \lambda \in \mathbb{R}_{++}\}$ and the following are equivalent:*

- A is irreducible with respect to $\tilde{\mathcal{N}}^2$,
- $A = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$,
- $\mathcal{V}^A = \{\lambda \mathbf{e}_{12} \mid \lambda \in \mathbb{R}_{++}\}$.

Proof. For any $\mathbf{u} \in \mathbb{R}_+^2$ we have that $\mathbf{u}^\top A \mathbf{u} = u_1^2 + 2a_{12}u_1u_2 + u_2^2 = (u_1 - u_2)^2 + 2u_1u_2(a_{12} + 1)$. Hence, for A to be copositive, we must have that $a_{12} \geq -1$. We also see that $\mathbf{u} \in \mathcal{V}^A$ if and only if $u_1 = u_2 > 0$ and $a_{12} = -1$. Now the fact that a matrix is irreducible with respect to $\tilde{\mathcal{N}}^n$ if and only if Property 3.10 holds gives us the required results. \square

The following corollary of this lemma is a consequence of the fact that all principal submatrices of a copositive matrix must be copositive, see property (ii) of Proposition 1.3.

Corollary 3.15. *Consider $A \in \mathcal{COP}^n$ with $\text{diag } A = \mathbf{e}$ and let $\mathbf{u} \in \mathcal{V}^A$ be such that $\text{supp}(\mathbf{u}) = \{i, j\}$ for some $i, j \in \{1, \dots, n\}$ with $i \neq j$. Then $a_{ij} = -1$ and there exists $\lambda \in \mathbb{R}_{++}$ such that $\mathbf{u} = \lambda \mathbf{e}_{ij}$.*

We now momentarily consider the following lemma.

Lemma 3.16. *Let $A \in \mathcal{COP}^n$ with $\text{diag } A = \mathbf{e}$ be irreducible with respect to $\tilde{\mathcal{N}}^n$. Then $a_{ij} \in [-1, 1]$ for all $i, j = 1, \dots, n$.*

Proof. Consider $A \in \mathcal{COP}^n$ such that $\text{diag } A = \mathbf{e}$. All order 2 principle submatrices of A must be copositive, which implies that $a_{ij} \geq -1$ for all $i, j = 1, \dots, n$. Now considering work done on the copositive completion problem [HJR05] we see that all off-diagonal elements of A which are strictly greater than 1 can have their value replaced by 1 and the matrix would remain to be copositive. Therefore if A is irreducible with respect to $\tilde{\mathcal{N}}^n$, then we must have that $a_{ij} \leq 1$ for all $i, j = 1, \dots, n$. \square

Combining this lemma with Corollary 3.15 and noting that all order 3 principal submatrices of a copositive matrix must be in $\mathcal{COP}^3 = \mathcal{S}_+^3 + \mathcal{N}^3$ gives us the following result.

Lemma 3.17. *Let $A \in \mathcal{COP}^n$ be irreducible with respect to $\tilde{\mathcal{N}}^n$ and $\text{diag } A = \mathbf{e}$. Suppose $\{i, j\}, \{j, k\} \in \text{supp } (\mathcal{V}^A)$, where i, j, k are mutually different. Then $A_{\{i,j,k\}}$ is a rank 1 positive semidefinite matrix with $1 = a_{ik} = -a_{ij} = -a_{jk}$.*

Next we consider order 3 copositive matrices specifically.

Lemma 3.18. *A matrix $A \in \mathcal{COP}^3$ with $\text{diag } A = \mathbf{e}$ is irreducible with respect to $\tilde{\mathcal{N}}^3$ if and only if it can be represented in the form*

$$A = \begin{pmatrix} 1 & -\cos \zeta & \cos(\zeta + \xi) \\ -\cos \zeta & 1 & -\cos \xi \\ \cos(\zeta + \xi) & -\cos \xi & 1 \end{pmatrix} \quad (3.6)$$

for some $(\zeta, \xi) \in \Psi := \{(\zeta, \xi) \in \mathbb{R}_+^2 \mid \zeta + \xi \leq \pi\}$.

We have that $\text{supp } (\mathcal{V}^A) = \{\{1, 2, 3\}\}$ if and only if $(\zeta, \xi) \in \text{int}(\Psi)$. In this case the zero is proportional to $(\sin \xi, \sin(\zeta + \xi), \sin \zeta)^\top$.

Proof. Before we begin this proof, first note that a matrix A of the form (3.6) can be decomposed as

$$A = \begin{pmatrix} -\cos \zeta \\ 1 \\ -\cos \xi \end{pmatrix} \begin{pmatrix} -\cos \zeta \\ 1 \\ -\cos \xi \end{pmatrix}^\top + \begin{pmatrix} \sin \zeta \\ 0 \\ -\sin \xi \end{pmatrix} \begin{pmatrix} \sin \zeta \\ 0 \\ -\sin \xi \end{pmatrix}^\top \in \mathcal{S}_+^3 \subset \mathcal{COP}^3. \quad (3.7)$$

Now let us show that if $A \in \mathcal{COP}^3$ with $\text{diag } A = \mathbf{e}$ is irreducible with respect to $\tilde{\mathcal{N}}^3$ then it must be represented in the required form. From Lemma 3.16 we see that there must exist $\zeta, \xi \in [0, \pi]$ and $a_{13} \in [-1, 1]$ such that

$$A = \begin{pmatrix} 1 & -\cos \zeta & a_{13} \\ -\cos \zeta & 1 & -\cos \xi \\ a_{13} & -\cos \xi & 1 \end{pmatrix}.$$

As A is irreducible with respect to $\tilde{\mathcal{N}}^3$, we must have that $\mathcal{V}^A \neq \emptyset$, and thus

$$0 = \det A = -(a_{13} - \cos \zeta \cos \xi)^2 + \sin^2 \zeta \sin^2 \xi.$$

Therefore $a_{13} = \cos \zeta \cos \xi \pm \sin \zeta \sin \xi$. For both possible values of a_{13} we would get that the matrix A is positive semidefinite, and thus copositive. Therefore A being irreducible with respect to $\tilde{\mathcal{N}}^3$ means that

$$a_{13} = \min\{\cos \zeta \cos \xi \pm \sin \zeta \sin \xi\} = \cos \zeta \cos \xi - \sin \zeta \sin \xi = \cos(\zeta + \xi).$$

We are now left to show that $\zeta + \xi \leq \pi$. Suppose for the sake of contradiction that $\zeta + \xi > \pi$. We must have that $\zeta, \xi > 0$. Assuming $\zeta = \xi = \pi$ would

give that A is the matrix with all entries equal to one, which is clearly not irreducible with respect to $\tilde{\mathcal{N}}^3$. Therefore $\zeta + \xi < 2\pi$ and w.l.o.g. assume $\zeta \in (0, \pi)$. This implies that the vectors $(-\cos \zeta, 1, -\cos \xi)^\top$ and $(\sin \zeta, 0, -\sin \xi)^\top$ from (3.7) are linearly independent and so we get that

$$\begin{aligned} \emptyset \neq \mathcal{V}^A &= \mathbb{R}_+^3 \cap \left\{ \mathbf{x} \in \mathbb{R}^3 \mid 0 = \mathbf{x}^\top \begin{pmatrix} -\cos \zeta \\ 1 \\ -\cos \xi \end{pmatrix} = \mathbf{x}^\top \begin{pmatrix} \sin \zeta \\ 0 \\ -\sin \xi \end{pmatrix} \right\} \setminus \{\mathbf{0}\} \\ &= \mathbb{R}_+^3 \cap \left\{ \lambda \begin{pmatrix} \sin \xi \\ \sin(\zeta + \xi) \\ \sin \zeta \end{pmatrix} \mid \lambda \in \mathbb{R} \setminus \{0\} \right\} \\ &= \emptyset. \end{aligned}$$

This gives us our contradiction, and so if $A \in \mathcal{COP}^3$ with $\text{diag } A = \mathbf{e}$ is irreducible with respect to $\tilde{\mathcal{N}}^3$ then it must be representable in the required form.

Next we show that any matrix of the form (3.6) is irreducible with respect to $\tilde{\mathcal{N}}^3$. From the decomposition (3.7) we see that it is positive semidefinite, and hence copositive. If $\zeta = 0$ then $A\mathbf{e}_{12} = \mathbf{0}$ and so A is irreducible with respect to $\tilde{\mathcal{N}}^3$ by Theorem 3.8. Similar reasoning holds for $\xi = 0$ and for $\zeta + \xi = \pi$, so we are left to consider $(\zeta, \xi) \in \text{int}(\Psi)$. In this case we have that $\mathbf{u} := (\sin \xi, \sin(\zeta + \xi), \sin \zeta)^\top \in \mathcal{V}^A$ is a strictly positive vector, $A\mathbf{u} = \mathbf{0}$, and so again by Theorem 3.8 we have that A is irreducible with respect to $\tilde{\mathcal{N}}^3$.

Finally from this discussion it is trivial to prove the last result for $\text{supp}(\mathcal{V}^A) = \{\{1, 2, 3\}\}$. □

From the last lemma we get the following corollary.

Corollary 3.19. *Let $A \in \mathcal{COP}^3$ with $\text{diag } A = \mathbf{e}$ and $a_{13} = 1$ be irreducible with respect to $\tilde{\mathcal{N}}^3$. Then $a_{12} = a_{23} = -1$ so that $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{2, 3\}, \{1, 2, 3\}\}$.*

The main work of the following section will be on classifying matrices in \mathcal{COP}^5 which are irreducible with respect to $\tilde{\mathcal{N}}^5$. Before we begin this, however, we will first need a few more auxilliary results.

Lemma 3.20 (Lemma 3.1 of [Bau66]). *Let $A \in \mathcal{COP}^n$ and $\mathbf{u} \in \mathcal{V}^A$ be such that $A\mathbf{u} = \mathbf{0}$. Let $\mathcal{I} = \text{supp}(\mathbf{u})$. Then $A = P + C$, where $P \in \mathcal{S}_+^n$ is such that the rank of P equals the rank of the submatrix $P_{\mathcal{I}}$, and $C \in \mathcal{COP}^n$ is such that $c_{ij} = 0$ for all $i, j = 1, \dots, n$ such that $j \in \mathcal{I}$.*

This important lemma has several consequences.

Corollary 3.21 (Corollary 3.2 of [Bau66]). *Let $A \in \mathcal{COP}^n$ and let $\mathbf{u} \in \mathcal{V}^A$ be such that $|\text{supp}(\mathbf{u})| = n - 1$ and $A\mathbf{u} = \mathbf{0}$. Then $A \in \mathcal{S}_+^n$.*

The following corollary comes trivially from combining Lemmas 3.13 and 3.20.

Corollary 3.22. *Let $A \in \mathcal{COP}^5$ be irreducible with respect to $\tilde{\mathcal{N}}^5$ and $\mathbf{u} \in \mathcal{V}^A$ be such that $A\mathbf{u} = \mathbf{0}$. Then $A \in \mathcal{S}_+^5$.*

Next we consider the following lemma whose proof is similar to that of [Dia62, Lemma 11].

Lemma 3.23. *Let $A \in \mathcal{COP}^n$ be irreducible with respect to $\tilde{\mathcal{N}}^n$, and assume there is an $(n - 1) \times (n - 1)$ principal submatrix B of A which is positive semidefinite. Then $A \in \mathcal{S}_+^n$.*

Proof. Assume w.l.o.g. that B is the upper left subblock and partition A as

$$A = \begin{pmatrix} B & \mathbf{a} \\ \mathbf{a}^\top & \mu \end{pmatrix} \quad \text{with } B \in \mathcal{S}_+^{n-1}, \mathbf{a} \in \mathbb{R}^{n-1}, \mu \in \mathbb{R}_+.$$

Let $\gamma \geq 0$ be the largest number such that $\tilde{A} := A - \gamma E_{\{nn\}} \in \mathcal{COP}^n$ and set $\tilde{\mu} := \mu - \gamma$. Then \tilde{A} is irreducible with respect to $E_{\{nn\}}$, and by [Bau66, Theorem 3.4] there exists $\tilde{\mathbf{u}} \in \mathbb{R}_+^{n-1}$ such that $\mathbf{u} = (\tilde{\mathbf{u}}^\top, 1)^\top$ is a zero of \tilde{A} . By Lemma 3.5 we then have

$$\tilde{A}\mathbf{u} = \begin{pmatrix} B\tilde{\mathbf{u}} + \mathbf{a} \\ \mathbf{a}^\top \tilde{\mathbf{u}} + \tilde{\mu} \end{pmatrix} \geq \mathbf{0}.$$

Moreover, by Lemma 3.7 we have that $(\tilde{A}\mathbf{u})_k = 0$ for all $k \in \text{supp}(\mathbf{u})$. In particular, $0 = (\tilde{A}\mathbf{u})_n = \mathbf{a}^\top \tilde{\mathbf{u}} + \tilde{\mu}$ and $0 = \mathbf{u}^\top \tilde{A}\mathbf{u} - (\tilde{A}\mathbf{u})_n = \tilde{\mathbf{u}}^\top B\tilde{\mathbf{u}} + \mathbf{a}^\top \tilde{\mathbf{u}} = 0$. Therefore

$$A = \begin{pmatrix} B & -B\tilde{\mathbf{u}} \\ (-B\tilde{\mathbf{u}})^\top & \tilde{\mathbf{u}}^\top B\tilde{\mathbf{u}} \end{pmatrix} + \begin{pmatrix} 0 & B\tilde{\mathbf{u}} + \mathbf{a} \\ (B\tilde{\mathbf{u}} + \mathbf{a})^\top & \gamma \end{pmatrix}$$

which is the sum of a positive semidefinite matrix and a nonnegative matrix. The proof is concluded by Lemma 3.13. \square

Combining this lemma with Lemma 3.13 and $\mathcal{S}_+^4 + \mathcal{N}^4 = \mathcal{COP}^4$ [Dia62, Theorem 2] gives us the following corollary.

Corollary 3.24. *Let $A \in \mathcal{COP}^5$ be irreducible with respect to $\tilde{\mathcal{N}}^5$, and let some 4×4 submatrix B of A be irreducible with respect to $\tilde{\mathcal{N}}^4$. Then $A \in \mathcal{S}_+^5$.*

Corollary 3.24 is an analogue of [Bau67, Lemma 4.4], where this assertion has been proven for irreducibility with respect to \mathcal{N}^n .

Corollary 3.25. *Let $A \in \mathcal{COP}^n$ be irreducible with respect to $\tilde{\mathcal{N}}^n$. If there exists $\mathbf{u} \in \mathcal{V}^A$ such that $|\text{supp}(\mathbf{u})| \geq n - 1$, then $A \in \mathcal{S}_+^n$.*

Proof. If A has a zero with n positive components, then A is positive semidefinite by [Dia62, Lemma 7, (i)]. If A has a zero with $n - 1$ positive components, then the corresponding principal submatrix is positive semidefinite by [Dia62, Lemma 7, (i)] and A is positive semidefinite by Lemma 3.23. \square

Corollary 3.26. *Let $A \in \mathcal{COP}^n$ be irreducible with respect to $\tilde{\mathcal{N}}^n$. If for $i \neq j$, $E_{\{ij\}}$ is associated to a zero \mathbf{u} with $|\text{supp}(\mathbf{u})| \geq n - 2$ and satisfying $u_i u_j = 0$, then $A \in \mathcal{S}_+^n$.*

Proof. Assume the condition of the corollary and let $\mathcal{I} = \text{supp}(\mathbf{u})$. Define $\mathcal{I}' = \mathcal{I} \cup \{i, j\}$. Since $u_i u_j = 0$, but $u_i + u_j > 0$, the index set \mathcal{I}' has at least $n - 1$ elements. Moreover, by Definition 3.9 for association and by Lemma 3.7, we have $(A\mathbf{u})_k = 0$ for all $k \in \mathcal{I}'$, and therefore $A_{\mathcal{I}'}$ is positive semidefinite by Corollary 3.21. The proof is concluded by Lemma 3.23. \square

We finish this section with the following corollary.

Corollary 3.27. *Let $A \in \mathcal{COP}^5 \setminus \mathcal{S}_+^5$ with $\text{diag } A = \mathbf{e}$ be irreducible with respect to $\tilde{\mathcal{N}}^5$. Then every zero of A either has exactly 2 or exactly 3 positive components. If (i, j) is such that $u_i u_j = 0$ for all $\mathbf{u} \in \mathcal{V}^A$, then $E_{\{ij\}}$ is associated to a zero \mathbf{e}_{kl} with $k \in \{i, j\}$ and $l \notin \{i, j\}$, and $0 = a_{ik} + a_{il} = a_{jk} + a_{jl}$.*

Proof. By Corollary 3.25, A cannot have a zero with more than 3 positive components. On the other hand, $\text{diag } A = \mathbf{e}$ contradicts the existence of zeros with exactly one positive component.

Now if (i, j) is such that $u_i u_j = 0$ for all $\mathbf{u} \in \mathcal{V}^A$, then by Corollary 3.26, $E_{\{ij\}}$ cannot be associated to a zero with 3 positive components. Hence $E_{\{ij\}}$ is associated to a zero with precisely 2 positive components, which must have the support described in the assertion of the corollary and the condition $\text{diag } A = \mathbf{e}$ ensures it is proportional to \mathbf{e}_{kl} , so it can be taken equal to. Finally by Definition 3.9 for association we have that $a_{ik} + a_{il} = a_{jk} + a_{jl} = 0$. \square

3.5 Classification of 5×5 copositive matrices

In this section we study matrices $A \in \mathcal{COP}^5$ which are irreducible with respect to $\tilde{\mathcal{N}}^5$.

Let us first consider the case of A having a zero diagonal entry, say $a_{55} = 0$. Then for $k = 1, \dots, 4$ we have by copositivity of A that $a_{k5} \geq 0$, and by

irreducibility w.r.t. $E_{\{k5\}}$ we must have $a_{k5} = 0$. Hence A effectively is a copositive 4×4 matrix augmented with a zero row and column, which implies $A \in \mathcal{S}_+^5 + \mathcal{N}^5$ by [Dia62, Theorem 2]. By Lemma 3.13 we then have that A is positive semidefinite.

We may therefore assume that all diagonal elements of A are strictly positive. By possibly conjugating A with a positive definite diagonal matrix, we may assume without loss of generality that $\text{diag } A = \mathbf{e}$. We next study irreducibility with respect to \mathcal{N}^5 , first when Property 3.4 does hold, and then when it does not.

3.5.1 Property 3.4

In [Bau67] the zero patterns of irreducible matrices in \mathcal{COP}^5 which satisfy Property 3.4 have been classified. The result is summarized in the following lemma.

Lemma 3.28 (pp. 10–15 of [Bau67]). *Let $A \in \mathcal{COP}^5$ have $\text{diag } A = \mathbf{e}$ and suppose A satisfies Property 3.4. Then either*

- (a) A is positive semidefinite, or
- (b) A is in the orbit of the Horn matrix H , or
- (c) there exists a relabeling of variables such that

$$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{3, 4, 5\}\} \subseteq \text{supp}(\mathcal{V}^A),$$

or

- (d) there exists a relabeling of variables such that

$$\{\{1, 2, 3\}, \{2, 3, 4\}, \{3, 4, 5\}, \{1, 4, 5\}, \{1, 2, 5\}\} = \text{supp}(\mathcal{V}^A).$$

We shall now analyse this in detail and show that, in fact, case (c) is a subcase of (a), and case (d) means that A is in the orbit of some $S(\boldsymbol{\theta})$ from (3.5). We start with case (c).

Lemma 3.29. *Let $A \in \mathcal{COP}^5$ with $\text{diag } A = \mathbf{e}$ be such that*

$$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{3, 4, 5\}\} \subseteq \text{supp}(\mathcal{V}^A)$$

Then A is positive semidefinite.

Proof. By Theorem 3.8 the matrix A and its submatrices $A_{\{1,2,3\}}$, $A_{\{1,2,4\}}$, $A_{\{1,2,5\}}$ and $A_{\{3,4,5\}}$ are irreducible with respect to $\tilde{\mathcal{N}}^5$ resp. $\tilde{\mathcal{N}}^3$ and by Lemma 3.6 these submatrices are positive semidefinite. By Lemma 3.18 we then have

$$A = \begin{pmatrix} 1 & -\cos \theta_1 & \cos(\theta_1 + \theta_2) & \cos(\theta_1 + \theta_3) & \cos(\theta_1 + \theta_4) \\ -\cos \theta_1 & 1 & -\cos \theta_2 & -\cos \theta_3 & -\cos \theta_4 \\ \cos(\theta_1 + \theta_2) & -\cos \theta_2 & 1 & -\cos \theta_5 & \cos(\theta_5 + \theta_6) \\ \cos(\theta_1 + \theta_3) & -\cos \theta_3 & -\cos \theta_5 & 1 & -\cos \theta_6 \\ \cos(\theta_1 + \theta_4) & -\cos \theta_4 & \cos(\theta_5 + \theta_6) & -\cos \theta_6 & 1 \end{pmatrix}$$

with

$$\theta \in \mathbb{R}_+^6, \quad \theta_1 + \theta_2 \leq \pi, \quad \theta_1 + \theta_3 \leq \pi, \quad \theta_1 + \theta_4 \leq \pi, \quad \theta_5 + \theta_6 \leq \pi.$$

We shall now split the remainder of this proof in to three cases:

Case 1: $\theta_1 = 0$. It can be immediately seen that $\mathbf{e}_{12} \in \mathcal{V}^A$ and $A\mathbf{e}_{12} = \mathbf{0}$. Therefore Corollary 3.22 implies that A must be positive semidefinite.

Case 2: $\theta_1 = \pi$. From the inequalities on θ we have that $0 = \theta_2 = \theta_3 = \theta_4$. We then get that $\mathbf{e}_{1k} \in \mathcal{V}^A$ for $k = 3, 4, 5$. From considering Lemma 3.5 we see that for $k, m = 3, 4, 5$ we have that $0 \leq (A\mathbf{e}_{1k})_m = a_{1m} + a_{km} = -1 + a_{km}$. Therefore $a_{km} \geq 1$ for all $k, m = 3, 4, 5$, which by looking at the form of A gives us a contradiction and so this case is not possible.

Case 3: $0 < \theta_1 < \pi$. From the inequalities on θ we have that $0 \leq \theta_2, \theta_3, \theta_4 < \pi$ and $0 \leq \theta_5, \theta_6, (\theta_5 + \theta_6) \leq \pi$.

If we let $\mathbf{u} := (\sin \theta_2, \sin(\theta_1 + \theta_2), \sin \theta_1, 0, 0)^\top$ and $\mathbf{v} := (\sin \theta_3, \sin(\theta_1 + \theta_3), 0, \sin \theta_1, 0)^\top$, then we have that $\mathbf{u}, \mathbf{v} \in \mathcal{V}^A$ and therefore by Lemma 3.5 $A\mathbf{u} \geq \mathbf{0}$ and $A\mathbf{v} \geq \mathbf{0}$. Specifically from using standard trigonometric identities we get that

$$0 \leq (A\mathbf{u})_4 = -2 \sin \theta_1 \cos\left(\frac{1}{2}(|\theta_2 - \theta_3| + \theta_5)\right) \cos\left(\frac{1}{2}(|\theta_2 - \theta_3| - \theta_5)\right).$$

We have $0 < \theta_1 < \pi$ and $0 \leq |\theta_2 - \theta_3| < \pi$ and $0 \leq \theta_5 \leq \pi$, and combining these with the inequalities above gives us that $|\theta_2 - \theta_3| \geq \pi - \theta_5$. Similarly by considering $(A\mathbf{u})_5$ we get that $|\theta_2 - \theta_4| \geq \theta_5 + \theta_6$ and by considering $(A\mathbf{v})_5$ we see that $|\theta_3 - \theta_4| \geq \pi - \theta_6$. Adding these new inequalities together we get

$$2\pi \leq |\theta_2 - \theta_3| + |\theta_2 - \theta_4| + |\theta_3 - \theta_4| = 2 \max\{|\theta_2 - \theta_3|, |\theta_2 - \theta_4|, |\theta_3 - \theta_4|\} < 2\pi,$$

a contradiction, so this case is not possible either. \square

Next, we study case (d) of Lemma 3.28.

Lemma 3.30. *Let $A \in \mathcal{COP}^5$ with $\text{diag } A = \mathbf{e}$ be such that*

$$\{\{1, 2, 3\}, \{2, 3, 4\}, \{3, 4, 5\}, \{1, 4, 5\}, \{1, 2, 5\}\} = \text{supp}(\mathcal{V}^A).$$

Then $A = S(\boldsymbol{\theta})$ with $\boldsymbol{\theta} \in \mathbb{R}_{++}^5$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$.

Proof. By considering Lemma 3.18 and Theorem 3.8 we can immediately see that $A = S(\boldsymbol{\theta})$ with $\boldsymbol{\theta} \in \mathbb{R}_{++}^5$ and $\theta_i + \theta_{(i+1) \bmod 5} < \pi$ for all $i = 1, \dots, 5$. We are now left to show that $\mathbf{e}^\top \boldsymbol{\theta} < \pi$.

First suppose that $\mathbf{e}^\top \boldsymbol{\theta} = \pi$. Then we have that

$$S(\boldsymbol{\theta}) = \begin{pmatrix} \cos(\theta_1 + \theta_2) \\ -\cos \theta_2 \\ 1 \\ -\cos \theta_3 \\ \cos(\theta_3 + \theta_4) \end{pmatrix} \begin{pmatrix} \cos(\theta_1 + \theta_2) \\ -\cos \theta_2 \\ 1 \\ -\cos \theta_3 \\ \cos(\theta_3 + \theta_4) \end{pmatrix}^\top + \begin{pmatrix} \sin(\theta_1 + \theta_2) \\ -\sin \theta_2 \\ 1 \\ \sin \theta_3 \\ -\sin(\theta_3 + \theta_4) \end{pmatrix} \begin{pmatrix} \sin(\theta_1 + \theta_2) \\ -\sin \theta_2 \\ 1 \\ \sin \theta_3 \\ -\sin(\theta_3 + \theta_4) \end{pmatrix}^\top,$$

and from this we would get more than the required zeros, and thus $\mathbf{e}^\top \boldsymbol{\theta} = \pi$ is not possible.

Now suppose that $\mathbf{e}^\top \boldsymbol{\theta} > \pi$. We must have $\mathbf{e}^\top \boldsymbol{\theta} = \frac{1}{2} \sum_{i=1}^5 (\theta_i + \theta_{(i+1) \bmod 5}) < \frac{5\pi}{2}$. As A is copositive, any order 4 principal submatrix of A must be copositive. We can in fact consider an arbitrary order 4 principal submatrix of A and then extend any results from this specific case to all order 4 principal submatrices of A by cycling the indices. So consider $\tilde{A} := A_{\{1,2,3,4\}}$ and $\mathbf{x} := (\sin \theta_2, \sin(\theta_1 + \theta_2), \sin \theta_1, 0)^\top$. Then $\mathbf{x} \in \mathcal{V}^{\tilde{A}}$ and therefore by Lemma 3.5 we have that $\tilde{A}\mathbf{x} \geq \mathbf{0}$. In particular, using standard trigonometric identities, we get that

$$0 \leq (\tilde{A}\mathbf{x})_4 = 2 \sin \theta_2 \cos\left(\frac{1}{2}(\mathbf{e}^\top \boldsymbol{\theta})\right) \cos\left(\frac{1}{2}(\theta_1 + \theta_2 + \theta_3 - \theta_4 - \theta_5)\right).$$

We have that $0 < \theta_2 < \pi$ which implies that $\sin \theta_2 > 0$. We also have that $\frac{\pi}{2} < \frac{1}{2}(\mathbf{e}^\top \boldsymbol{\theta}) < \frac{5\pi}{4}$ which implies that $\cos\left(\frac{1}{2}(\mathbf{e}^\top \boldsymbol{\theta})\right) < 0$. This means that $\cos\left(\frac{1}{2}(\theta_1 + \theta_2 + \theta_3 - \theta_4 - \theta_5)\right) \leq 0$ which combined with the fact that $-\frac{\pi}{2} < \frac{1}{2}(\theta_1 + \theta_2 + \theta_3 - \theta_4 - \theta_5) < \frac{3\pi}{4}$ gives us that $\theta_1 + \theta_2 + \theta_3 - \theta_4 - \theta_5 \geq \pi$. We can now extend this result by cycling the indices to give us that

$$\theta_i + \theta_{(i+1) \bmod 5} + \theta_{(i+2) \bmod 5} - \theta_{(i+3) \bmod 5} - \theta_{(i+4) \bmod 5} \geq \pi \quad \text{for all } i = 1, \dots, 5.$$

Adding these inequalities together then gives us the contradiction that $\mathbf{e}^\top \boldsymbol{\theta} \geq 5\pi$. \square

We can now summarize the results of this subsection in to the following theorem.

Theorem 3.31. *Let $A \in \mathcal{COP}^5$ satisfy Property 3.4. Then either A is positive semidefinite, or A is in the orbit of $S(\boldsymbol{\theta})$ with $\boldsymbol{\theta} \in \mathbb{R}_{++}^5 \cup \{\mathbf{0}\}$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$.*

3.5.2 Property 3.10 but not Property 3.4

In this subsection we study when a matrix $A \in \mathcal{COP}^5$ is irreducible with respect to $\tilde{\mathcal{N}}^5$ but does not satisfy Property 3.4, or in other words it satisfies Property 3.10 but not Property 3.4. The main result of this section will be to show that every such matrix must either be positive semidefinite or in the orbit of some $S(\boldsymbol{\theta})$ described in Theorem 3.11, i.e., a matrix $S(\boldsymbol{\theta})$ as in (3.5) with $\boldsymbol{\theta} \in \mathbb{R}_+^5 \setminus (\mathbb{R}_{++}^5 \cup \{\mathbf{0}\})$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$.

In order to prove this we shall assume, for the sake of contradiction, that there exists $A \in \mathcal{COP}^5$ such that A is irreducible with respect to $\tilde{\mathcal{N}}^5$, Property 3.4 does not hold and A is neither positive semidefinite nor in the orbit of one of the matrices enumerated in Theorem 3.11. From the comment at the start of Section 3.5 we may again assume without loss of generality that $\text{diag } A = \mathbf{e}$.

By Corollary 3.27, the zeros of A have exactly 2 or 3 positive components. Both types of zeros can be represented as edges in a graph with 5 vertices. We will represent a zero with support $\{i, j\}$ by a dashed edge between the vertices i and j , whilst we will represent a zero with support $\{1, \dots, 5\} \setminus \{i, j\}$ by a solid edge between the vertices i and j . We have that the graph of the zeros of A must fulfill the following conditions:

1. *For every vertex i there exist vertices j, k such that i, j, k are pairwise distinct, j, k are not linked by a dashed edge, and every solid edge having i as one of its vertices must have either j or k as its other vertex.* If for some i such vertices j, k do not exist, then the 4×4 submatrix obtained from A by crossing out row and column i satisfies Property 3.4. As a consequence, it satisfies also the weaker Property 3.10, and hence A is positive semidefinite by Theorem 3.8 and Corollary 3.24. In particular, *no three solid edges can join in a vertex, and no triangle consisting of two solid and one dashed edge is possible.*

2. *There exist distinct vertices i, j , not joined by a dashed edge, such that every solid edge has at least one of i, j as one of its vertices.* If such a pair i, j does not exist, then A satisfies Property 3.4.

3. *If two dashed edges join in a vertex, then the two vertices which do not intersect one of these dashed edges are joined by a solid edge.* By Lemma 3.17 the sum of the zeros represented by the dashed edges is also a zero, represented by the solid edge.

4. *If there is a dashed edge (i, j) and a solid edge (k, l) such that i, j, k, l are pairwise distinct, then there is another dashed edge joining either i, m or j, m , where m is the remaining vertex.* The solid edge stands for a $\mathbf{v} \in \mathcal{V}^A$ with support $\{i, j, m\}$, implying that the submatrix $A_{\{i, j, m\}}$ is positive semidefinite. But then \mathbf{e}_{ij} and \mathbf{v} are linearly independent kernel vectors of $A_{\{i, j, m\}}$, and

$A_{\{i,j,m\}}$ is of rank 1. Existence of either a zero \mathbf{e}_{im} or \mathbf{e}_{jm} now easily follows.

5. *There are no dashed triangles.* If there were a dashed triangle on the vertices i, j, k , then the submatrix $A_{\{i,j,k\}}$ would have all off-diagonal elements equal to -1 and could not be in \mathcal{COP}^3 .

6. *There cannot exist pairwise distinct vertices i, j, k, l such that both (i, j) and (i, k) are dashed edges whilst (i, l) is a solid edge.* The existence of zeros $\mathbf{e}_{ij}, \mathbf{e}_{ik}$ implies by Lemma 3.17 that $a_{jk} = 1$. Since A has a zero with support $\{j, k, m\}$, where m is the remaining vertex, the submatrix $A_{\{j,k,m\}}$ is irreducible by Theorem 3.8. Existence of the zeros $\mathbf{e}_{jm}, \mathbf{e}_{km}$ now follows from Lemma 3.19. Now if we consider condition 3 we get $(j, l), (k, l)$ and (l, m) are solid edges. Finally considering condition 1, we get a contradiction.

7. *For every two distinct vertices i, j , either there exists a dashed edge with at least one of i, j as one of its vertices, or there exists a solid edge whose vertices are not in $\{i, j\}$.* If a dashed edge with the specified properties does not exist, then $E_{\{ij\}}$ is not associated to a zero with exactly 2 positive components. Hence $E_{\{ij\}}$ must be associated to a zero \mathbf{u} with 3 positive components, and by Corollary 3.27 this zero must satisfy $u_i u_j > 0$.

Applying these rules it can be found that the only graphs satisfying these conditions, up to permutation of the vertices, are given in Fig. 3.1. These give us 14 possible cases for A to consider, which we have ordered and permuted for ease of going through them. For each one we shall find a contradiction in the form of A being positive semidefinite or A being in the orbit of some $S(\boldsymbol{\theta})$ described in Theorem 3.11, i.e., $S(\boldsymbol{\theta})$ as in (3.5) with $\boldsymbol{\theta} \in \mathbb{R}_+^5 \setminus (\mathbb{R}_{++}^5 \cup \{\mathbf{0}\})$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$.

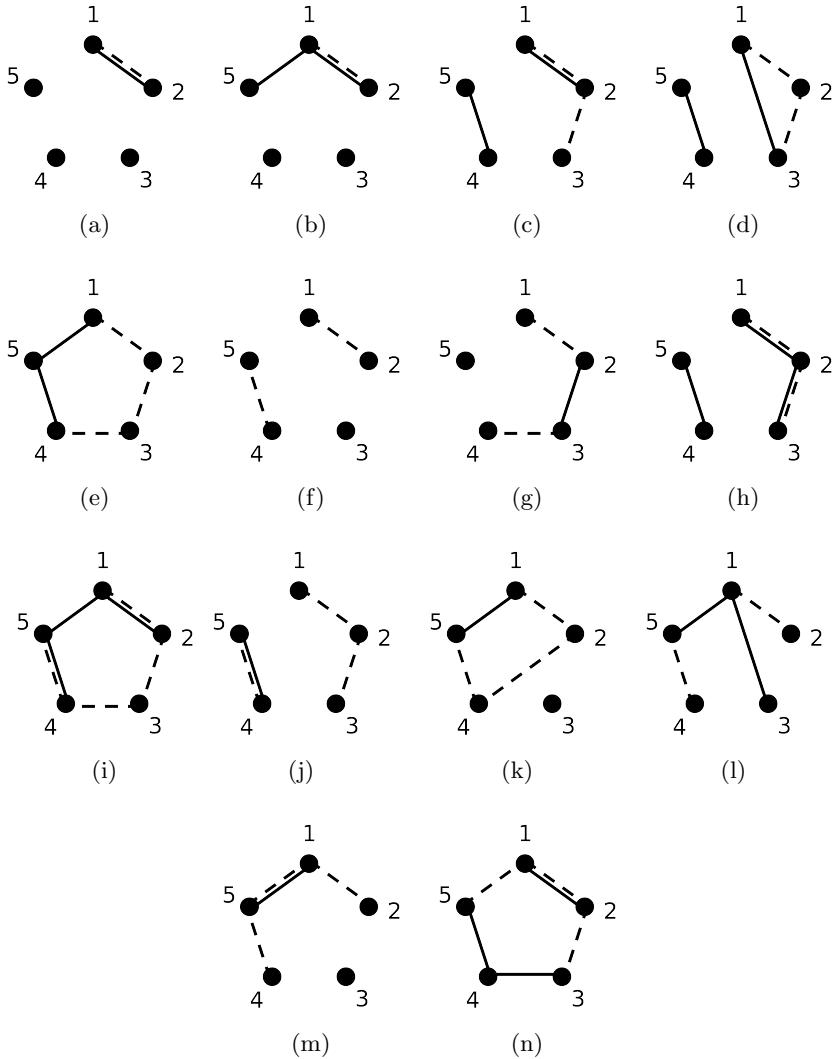


Figure 3.1: Graphs fulfilling the conditions in Subsection 3.5.2, used to represent the support of the set of zeros of a matrix. A dashed edge between vertices i and j represents a zero with support $\{i, j\}$, whilst a solid edge between the vertices i and j represents a zero with support $\{1, \dots, 5\} \setminus \{i, j\}$.

Before we do this however, we will first recall the following which we shall use regularly when going through these cases.

- By Corollary 3.15 we have that if $\{i, j\} \in \text{supp}(\mathcal{V}^A)$ with $i \neq j$, then up to positive scalings \mathbf{e}_{ij} is the unique zero with this support.

- By Lemma 3.7, for $\mathbf{u}, \mathbf{v} \in \mathcal{V}^A$ with $\text{supp}(\mathbf{u}) \subseteq \text{supp}(\mathbf{v})$ we have $(A\mathbf{u})_i = 0$ for all $i \in \text{supp}(\mathbf{v})$.
- By Corollary 3.22, there cannot exist $\mathbf{u} \in \mathcal{V}^A$ such that $A\mathbf{u} = \mathbf{0}$.
- By Corollary 3.27, if $i \neq j$ is such that $u_i u_j = 0$ for all $\mathbf{u} \in \mathcal{V}^A$, then $E_{\{ij\}}$ is associated to a zero \mathbf{e}_{kl} with $k \in \{i, j\}$ and $l \notin \{i, j\}$.
- By Lemma 3.16 we have that $a_{ij} \in [-1, 1]$ for all $i = 1, \dots, 5$.

We shall use these results regularly whilst going through the cases without specifically referencing them.

(a) $\text{supp}(\mathcal{V}^A) = \{\{3, 4, 5\}, \{1, 2\}\}$:

We have $(A\mathbf{e}_{12})_i = 0$ for $i = 1, 2$. For $k = 3, 4, 5$ we must have that $E_{\{1k\}}$ is associated to \mathbf{e}_{12} , and thus $\mathbf{0} = A\mathbf{e}_{12} \neq \mathbf{0}$.

(b) $\text{supp}(\mathcal{V}^A) = \{\{2, 3, 4\}, \{3, 4, 5\}, \{1, 2\}\}$:

By following the same steps as in the previous case, we again get a contradiction.

(c) $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{2, 3\}, \{1, 2, 3\}, \{3, 4, 5\}\}$:

We have $(A\mathbf{e}_{12})_i = 0$ for $i = 1, 2, 3$. We also have that both $E_{\{14\}}$ and $E_{\{15\}}$ must be associated to \mathbf{e}_{12} , hence $\mathbf{0} = A\mathbf{e}_{12} \neq \mathbf{0}$.

(d) $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{2, 3\}, \{1, 2, 3\}, \{2, 4, 5\}\}$:

By following the same steps as in the previous case, we again get a contradiction.

(e) $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{2, 3\}, \{3, 4\}, \{1, 2, 3\}, \{2, 3, 4\}\}$:

We must have that $E_{\{14\}}$ is associated to either \mathbf{e}_{12} or \mathbf{e}_{34} . Without loss of generality, let it be associated to \mathbf{e}_{12} , and so $(A\mathbf{e}_{12})_4 = 0$. However, we must also have $0 = (A\mathbf{e}_{12})_i$ for $i = 1, 2, 3$. Finally we have that $E_{\{15\}}$ must be associated to \mathbf{e}_{12} , implying $\mathbf{0} = A\mathbf{u}_{12} \neq \mathbf{0}$.

(f) $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{4, 5\}\}$:

Without loss of generality $E_{\{24\}}$ is associated to \mathbf{e}_{12} , implying $(A\mathbf{e}_{12})_4 = 0$. We must have that $E_{\{13\}}$ and $E_{\{34\}}$ are associated to \mathbf{e}_{12} and \mathbf{e}_{45} respectively, hence $0 = (A\mathbf{e}_{12})_3 = (A\mathbf{e}_{45})_3$. We must then have $(A\mathbf{e}_{12})_5 > 0$, otherwise $A\mathbf{e}_{12} = \mathbf{0}$. This however implies that both $E_{\{15\}}$ and $E_{\{25\}}$ must be associated to \mathbf{e}_{45} and so $\mathbf{0} = A\mathbf{e}_{45} \neq \mathbf{0}$.

(g) $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{3, 4\}, \{1, 4, 5\}\}$:

Without loss of generality $E_{\{23\}}$ is associated to \mathbf{e}_{12} , implying $0 = (A\mathbf{e}_{12})_3 = a_{13} + a_{23}$. Further, $E_{\{25\}}$ and $E_{\{35\}}$ are associated to \mathbf{e}_{12} and \mathbf{e}_{34} respectively, implying that $0 = (A\mathbf{e}_{12})_5 = a_{15} + a_{25}$ and $0 = (A\mathbf{e}_{34})_5 = a_{35} + a_{45}$. We must have $(A\mathbf{e}_{12})_4 > 0$, otherwise $A\mathbf{e}_{12} = \mathbf{0}$, and hence $E_{\{24\}}$ must be associated to \mathbf{e}_{34} , implying $0 = (A\mathbf{e}_{34})_2 = a_{23} + a_{24}$. From this and Lemma 3.18 we see that

$$A = \begin{pmatrix} 1 & -1 & a_{13} & \cos(\theta_4 + \theta_5) & -\cos \theta_5 \\ -1 & 1 & -a_{13} & a_{13} & \cos \theta_5 \\ a_{13} & -a_{13} & 1 & -1 & \cos \theta_4 \\ \cos(\theta_4 + \theta_5) & a_{13} & -1 & 1 & -\cos \theta_4 \\ -\cos \theta_5 & \cos \theta_5 & \cos \theta_4 & -\cos \theta_4 & 1 \end{pmatrix} = S(\boldsymbol{\theta})$$

for some $\boldsymbol{\theta} = (0, \theta_2, 0, \theta_4, \theta_5)$, where $0 < \theta_2, \theta_4, \theta_5, (\theta_4 + \theta_5) < \pi$. We now recall the inequality $0 < (A\mathbf{e}_{12})_4 = \cos(\theta_4 + \theta_5) + \cos \theta_2 = 2 \cos(\frac{1}{2}(\theta_2 + \theta_4 + \theta_5)) \cos(\frac{1}{2}(\theta_4 + \theta_5 - \theta_2))$, which implies $\pi > \theta_2 + \theta_4 + \theta_5 = \mathbf{e}^\top \boldsymbol{\theta}$, and thus A is of the form $S(\boldsymbol{\theta})$ as in Theorem 3.11.

(h) $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{2, 3\}, \{1, 2, 3\}, \{3, 4, 5\}, \{1, 4, 5\}\}$:

Without loss of generality we have that $E_{\{25\}}$ is associated to \mathbf{e}_{12} , implying $0 = (A\mathbf{e}_{12})_5 = a_{15} + a_{25}$. Note that $(A\mathbf{e}_{12})_i = 0$ for $i = 1, 2, 3$. Therefore $(A\mathbf{e}_{12})_4 > 0$, and hence $E_{\{24\}}$ must be associated to \mathbf{e}_{23} , implying $0 = (A\mathbf{e}_{23})_4 = a_{24} + a_{34}$. From this and Lemma 3.18 we now see that $A = S(\boldsymbol{\theta})$ for some $\boldsymbol{\theta} = (0, 0, \theta_3, \theta_4, \theta_5)^\top$ with $0 < \theta_3, \theta_4, \theta_5, (\theta_3 + \theta_4), (\theta_4 + \theta_5) < \pi$. We recall $0 < (A\mathbf{e}_{12})_4 = 2 \cos(\frac{1}{2}(\theta_3 + \theta_4 - \theta_5)) \cos(\frac{1}{2}(\theta_3 + \theta_4 + \theta_5))$ from which we get that $\pi > \theta_3 + \theta_4 + \theta_5 = \mathbf{e}^\top \boldsymbol{\theta}$, and thus A is of the form $S(\boldsymbol{\theta})$ as in Theorem 3.11.

(i) $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{2, 3\}, \{3, 4\}, \{4, 5\}, \{1, 2, 3\}, \{2, 3, 4\}, \{3, 4, 5\}\}$:

We have that

$$A = \begin{pmatrix} 1 & -1 & 1 & a_{14} & a_{15} \\ -1 & 1 & -1 & 1 & a_{25} \\ 1 & -1 & 1 & -1 & 1 \\ a_{14} & 1 & -1 & 1 & -1 \\ a_{15} & a_{25} & 1 & -1 & 1 \end{pmatrix} = S(\boldsymbol{\theta}) + \delta_1 E_{\{14\}} + \delta_2 E_{\{25\}}$$

for some $\boldsymbol{\theta} = (0, 0, 0, 0, \theta_5)^\top$ and $\boldsymbol{\delta} \in \mathbb{R}^2$, with $0 < \theta_5 \leq \pi$. Moreover, $0 \leq (A\mathbf{e}_{45})_1 = \delta_1$ and $0 \leq (A\mathbf{e}_{12})_5 = \delta_2$. Therefore A can be written as the sum of the nonnegative matrix $(\delta_1 E_{\{45\}} + \delta_2 E_{\{25\}})$ and the copositive matrix $S(\boldsymbol{\theta})$ from (3.5). As A is irreducible we must therefore have that

$\boldsymbol{\delta} = \mathbf{0}$, and thus A is either positive semidefinite or of the form $S(\boldsymbol{\theta})$ as in Theorem 3.11.

(j) $\text{supp}(\mathcal{V}^A) = \{\{1, 2\}, \{2, 3\}, \{4, 5\}, \{1, 2, 3\}\}$:

We have that $0 = (\mathbf{Ae}_{12})_i = (\mathbf{Ae}_{23})_i$ for $i = 1, 2, 3$. If both $E_{\{14\}}$ and $E_{\{15\}}$ are associated to \mathbf{e}_{12} then we would have that $\mathbf{Ae}_{12} = \mathbf{0}$. Therefore, without loss of generality $0 < (\mathbf{Ae}_{12})_4 = a_{14} + a_{24}$ and hence $E_{\{14\}}$ is associated to \mathbf{e}_{45} , implying that $0 = (\mathbf{Ae}_{45})_1 = a_{14} + a_{15}$. Similarly, we cannot have $0 = (\mathbf{Ae}_{23})_4 = (\mathbf{Ae}_{23})_5$, and hence there must be $k \in \{4, 5\}$ such that $(\mathbf{Ae}_{23})_k > 0$. But then $E_{\{3k\}}$ must be associated to \mathbf{e}_{45} , and $0 = (\mathbf{Ae}_{45})_3 = a_{34} + a_{35}$. $\mathbf{Ae}_{45} \neq \mathbf{0}$ then yields $0 < (\mathbf{Ae}_{45})_2$ and hence $E_{\{24\}}$ must be associated to \mathbf{e}_{23} , implying $0 = (\mathbf{Ae}_{23})_4 = a_{24} + a_{34}$. $\mathbf{Ae}_{23} \neq \mathbf{0}$ then yields $0 < (\mathbf{Ae}_{23})_5$, and hence $E_{\{25\}}$ must be associated to \mathbf{e}_{12} , implying $0 = (\mathbf{Ae}_{12})_5 = a_{15} + a_{25}$. Therefore

$$A = \begin{pmatrix} 1 & -1 & 1 & -a_{15} & a_{15} \\ -1 & 1 & -1 & -a_{34} & -a_{15} \\ 1 & -1 & 1 & a_{34} & -a_{34} \\ -a_{15} & -a_{34} & a_{34} & 1 & -1 \\ a_{15} & -a_{15} & -a_{34} & -1 & 1 \end{pmatrix} = S(\boldsymbol{\theta}),$$

for some $\boldsymbol{\theta} = (0, 0, \theta_3, 0, \theta_5)$ with $0 < \theta_3, \theta_5 \leq \pi$. We now recall the inequality $0 < a_{14} + a_{24} = 2 \cos(\frac{1}{2}(\theta_3 - \theta_5)) \cos(\frac{1}{2}(\theta_3 + \theta_5))$ which implies that $\pi > \theta_3 + \theta_5 = \mathbf{e}^\top \boldsymbol{\theta}$, and thus A is of the form $S(\boldsymbol{\theta})$ as in Theorem 3.11.

(k), (l), (m), (n) $\text{supp}(\mathcal{V}^A) \supseteq \{\{1, 5\}, \{1, 2, 3\}, \{3, 4, 5\}\}$:

By Lemma 3.18 we see that $A = S(\boldsymbol{\theta}) + \delta_1 E_{\{14\}} + \delta_2 E_{\{25\}} + \delta_3 E_{\{24\}}$, for some $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3, \theta_4, 0)^\top$ and $\boldsymbol{\delta} \in \mathbb{R}^3$ such that $0 \leq \theta_1, \theta_2, \theta_3, \theta_4, (\theta_1 + \theta_2), (\theta_3 + \theta_4) \leq \pi$. By Lemma 3.5 we have $0 \leq (\mathbf{Ae}_{15})_4 = \delta_1$ and $0 \leq (\mathbf{Ae}_{15})_2 = \delta_2$. Moreover we have that $0 \leq (\mathbf{Ae}_{15})_3 = 2 \cos(\frac{1}{2}(\theta_1 + \theta_2 - \theta_3 - \theta_4)) \cos(\frac{1}{2}(\theta_1 + \theta_2 + \theta_3 + \theta_4))$, implying that $\pi \geq \theta_1 + \theta_2 + \theta_3 + \theta_4 = \mathbf{e}^\top \boldsymbol{\theta}$. Also considering the copositivity of

$$A_{\{2,3,4\}} = \begin{pmatrix} 1 & -\cos \theta_2 & \cos(\theta_2 + \theta_3) + \delta_3 \\ -\cos \theta_2 & 1 & -\cos \theta_3 \\ \cos(\theta_2 + \theta_3) + \delta_3 & -\cos \theta_3 & 1 \end{pmatrix}$$

along with Lemma 3.18 and the constraint $\theta_2 + \theta_3 \leq \pi$ yields $\delta_3 \geq 0$. Therefore A can be written as the sum of the nonnegative matrix $(\delta_1 E_{\{14\}} + \delta_2 E_{\{25\}} + \delta_3 E_{\{24\}})$ and a copositive matrix in the orbit of some $S(\boldsymbol{\theta})$ from (3.5). As A is irreducible we must therefore have that $\boldsymbol{\delta} = \mathbf{0}$, and thus A is of the form $S(\boldsymbol{\theta})$ as in Theorem 3.11.

Summing up, we have proven the following result.

Theorem 3.32. *Let $A \in \mathcal{COP}^5$ be irreducible with respect to $\tilde{\mathcal{N}}^5$ and assume A does not satisfy Property 3.4. Then either A is positive semidefinite, or A is in the orbit of $S(\boldsymbol{\theta})$ with $\boldsymbol{\theta} \in \mathbb{R}_+^5 \setminus (\mathbb{R}_{++}^5 \cup \{\mathbf{0}\})$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$.*

3.5.3 Irreducible matrices of \mathcal{COP}^5

By combining Theorems 3.31 and 3.32, we obtain the following result.

Theorem 3.33. *Let $A \in \mathcal{COP}^5$ be irreducible with respect to $\tilde{\mathcal{N}}^5$. Then either A is positive semidefinite, or A is in the orbit of $S(\boldsymbol{\theta})$ given by (3.5) with $\boldsymbol{\theta} \in \mathbb{R}_+^5$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$.*

As being irreducible with respect to \mathcal{N}^5 is a stronger statement, this theorem must also hold for irreducibility with respect to \mathcal{N}^5 . The following theorem is also clear to see.

Theorem 3.34. *Let $A \in \mathcal{COP}^5$ be irreducible with respect to $\tilde{\mathcal{N}}^5$, but not irreducible with respect to \mathcal{N}^5 . Then A is positive semidefinite.*

Proof. Suppose for the sake of contradiction that there exists a matrix $A \in \mathcal{COP}^5 \setminus \mathcal{S}_+^5$ such that A is irreducible with respect to $\tilde{\mathcal{N}}^5$, but not irreducible with respect to \mathcal{N}^5 . It can be seen that A cannot satisfy Property 3.4, otherwise it would be irreducible with respect to \mathcal{N}^5 . Therefore, by Theorem 3.32 and $A \notin \mathcal{S}_+^5$, we get that A must be in the orbit of $S(\boldsymbol{\theta})$ with $\boldsymbol{\theta} \in \mathbb{R}_+^5 \setminus (\mathbb{R}_{++}^5 \cup \{\mathbf{0}\})$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$. However, by Theorem 3.11, this means that A is irreducible with respect to \mathcal{N}^5 , giving us a contradiction. \square

Our results immediately yield a simple characterization of those 5×5 copositive matrices which cannot be written as a sum of a positive semidefinite and a nonnegative matrix. Namely, we have the following result which, as mentioned before, can be seen as the dual statement to [BAD09, Corollary 2].

Corollary 3.35. *Let $A \in \mathcal{COP}^5 \setminus (\mathcal{S}_+^5 + \mathcal{N}^5)$. Then A can be expressed as $A = S + N$ for some $N \in \tilde{\mathcal{N}}^5$ and $S \in \mathcal{COP}^5$ in the orbit of $S(\boldsymbol{\theta})$ given by (3.5), where $\boldsymbol{\theta} \in \mathbb{R}_+^5$ and $\mathbf{e}^\top \boldsymbol{\theta} < \pi$.*