

# A New Certificate For Copositivity

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## Abstract

In this article, we introduce a new method of certifying any copositive matrix to be copositive. This is done through the use of a theorem by Haderler and the Farkas Lemma. For a given copositive matrix this certificate is constructed by solving finitely many linear systems, and can be subsequently checked by checking finitely many linear inequalities. In some cases, this certificate can be relatively small, even when the matrix generates an extreme ray of the copositive cone which is not positive semidefinite plus nonnegative. This certificate can also be used to generate the set of minimal zeros of a copositive matrix. In the final section of this paper we introduce a set of newly discovered extremal copositive matrices.

**Keywords:** Copositive Matrix; NP-hard; Certificate; Minimal zeros; Extreme ray

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## 1 Introduction

A symmetric matrix  $\mathbf{X} \in \mathcal{S}^n$  is copositive if  $\mathbf{v}^\top \mathbf{X} \mathbf{v} \geq 0$  for all entrywise nonnegative vectors  $\mathbf{v}$ . The set of copositive matrices of order  $n$  then forms a proper cone which is referred to as the copositive cone, denoted  $\mathcal{COP}^n$ , which is of interest for example in combinatorial optimisation [5, 7, 11, 18].

Checking copositivity is a co-NP-complete problem [32], i.e. checking copositivity is NP-hard, but if the matrix,  $\mathbf{X}$ , being checked is not copositive then there is a certificate for this which can be checked in polynomial time. This certificate is generally in the form of a rational nonnegative vector  $\mathbf{v}$  such that  $\mathbf{v}^\top \mathbf{X} \mathbf{v} < 0$ . The fact that checking copositivity is a co-NP-complete problem means that, in general, there cannot be a certificate which can certify a matrix to be copositive in polynomial time, unless co-NP = NP, which would contradict the conjecture that “co-NP  $\neq$  NP” [26, Chapter 11]<sup>1</sup>.

This does not mean that certificates for copositivity do not exist, it purely means that we should not expect them in general to be of polynomial size. As an example, it is a well known result that the sum of the positive semidefinite cone,  $\mathcal{PSD}^n$ , and the cone of nonnegative symmetric matrices,  $\mathcal{N}^n$ , is contained in the copositive cone, with

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<sup>1</sup>This is a stronger conjecture than its more famous cousin that “P  $\neq$  NP”, i.e. if co-NP  $\neq$  NP then this would imply that P  $\neq$  NP, but it may be possible that both co-NP = NP and P  $\neq$  NP.

it being shown in [9, 30] that  $\mathcal{PSD}^n + \mathcal{N}^n = \mathcal{COP}^n$  if and only if  $n \leq 4$ . If we have a matrix  $\mathbf{X} \in \mathcal{PSD}^n + \mathcal{N}^n$  then we could certify this by finding matrices  $\mathbf{A} \in \mathbb{R}^{n \times n}$  and  $\mathbf{B} \in \mathcal{N}^n$  such that  $\mathbf{X} = \mathbf{A}\mathbf{A}^\top + \mathbf{B}$ . An alternative way of certifying copositivity would be that if for  $m \in \mathbb{N}$  and  $\mathbf{X} \in \mathcal{S}^n$  we have that  $(\mathbf{1}_n^\top \mathbf{v})^m \mathbf{v}^\top \mathbf{X} \mathbf{v}$  is a polynomial in  $\mathbf{v}$  with all its coefficients nonnegative then this would also certify that  $\mathbf{X}$  is copositive (and if  $\mathbf{X}$  is in the interior of  $\mathcal{COP}^n$  then such a certificate always exists) [21, Section 2.24]. There are also plenty of other possible certificates of copositivity through for example moment matrices, sums-of-squares and simplicial partitions. We are unable to enumerate them all here and instead we direct the interested reader to [3, 6, 12, 14, 16, 17, 28, 33, 34] and [11, Part III].

These certificates are all limited in that they either do not work for all copositive matrices or they are difficult to construct and check.

The main result of this paper will be to give a new relatively simple certificate for copositivity, along with a method for finding such a certificate. This certificate works for all copositive matrices. It is constructed by (approximately) solving systems of linear equalities, and can be checked to confirm copositivity by checking linear inequalities. Due to the fact that checking copositivity is a co-NP-complete problem, in general this method would take exponential time to run and would produce an exponentially large certificate. For this reason we have not implemented the method, and instead we see this as a method for confirming special particular matrices of interest to be copositive.

## 2 Notation

We let  $\mathbb{N}$  be the set of strictly positive integers, and for  $n \in \mathbb{N}$  define  $[1:n] := \{1, \dots, n\}$  and  $\mathbb{P}[n] := \{\mathcal{I} \subseteq [1:n] : \mathcal{I} \neq \emptyset\}$ , e.g.

$$[1:3] = \{1, 2, 3\}, \quad \mathbb{P}[3] = \left\{ \{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}, \{1, 2, 3\} \right\}.$$

Note that the collection  $\mathbb{P}[n]$  is the power set of  $[1:n]$  excluding the empty set, and we have  $|\mathbb{P}[n]| = 2^n - 1$ .

We denote vectors in lower case bold, e.g.  $\mathbf{x}$ , and matrices in upper case, e.g.  $\mathbf{X}$ . We denote the  $i$ th entry of  $\mathbf{x}$  by  $x_i$ , and the  $(i, j)$  entry of  $\mathbf{X}$  by  $x_{ij}$ . For  $n \in \mathbb{N}$  define the vector and matrix sets:

$$\begin{aligned} \mathbb{R}^n &= \text{the set of real } n\text{-vectors,} \\ \mathbb{R}_+^n &= \{\mathbf{x} \in \mathbb{R}^n : x_i \geq 0 \forall i \in [1:n]\}, \\ \mathbb{R}_{++}^n &= \{\mathbf{x} \in \mathbb{R}^n : x_i > 0 \forall i \in [1:n]\}, \\ \mathcal{S}^n &= \{\mathbf{X} \in \mathbb{R}^{n \times n} : \mathbf{X} = \mathbf{X}^\top\}, \\ \mathcal{COP}^n &= \{\mathbf{X} \in \mathcal{S}^n : \mathbf{v}^\top \mathbf{X} \mathbf{v} \geq 0 \forall \mathbf{v} \in \mathbb{R}_+^n\}, \\ \mathcal{PSD}^n &= \{\mathbf{X} \in \mathcal{S}^n : \mathbf{v}^\top \mathbf{X} \mathbf{v} \geq 0 \forall \mathbf{v} \in \mathbb{R}^n\} = \{\mathbf{A}\mathbf{A}^\top : \mathbf{A} \in \mathbb{R}^{n \times n}\}, \\ \mathcal{N}^n &= \mathcal{S}^n \cap \mathbb{R}_+^{n \times n}, \\ \mathcal{SPN}^n &= \mathcal{PSD}^n + \mathcal{N}^n. \end{aligned}$$

For  $n \in \mathbb{N}$  we define  $\mathbf{1}_n \in \mathbb{R}^n$  (resp.  $\mathbf{0}_n \in \mathbb{R}^n$ ) to be the all ones (resp. all zeros) vector of order  $n$ , and for  $i \in [1:n]$  we define  $\mathbf{e}_i \in \mathbb{R}^n$  to be the unit vector with  $i$ th

entry equal to one and all other entries equal to zero (with the value of  $n$  apparent from the context).

For  $n \in \mathbb{N}$  and  $\mathbf{y} \in \mathbb{R}^n$  we define

$$\text{supp}(\mathbf{y}) := \{i \in [1:n] : y_i \neq 0\}, \quad \text{supp}_{\geq 0}(\mathbf{y}) := \{i \in [1:n] : y_i \geq 0\},$$

e.g. for  $\mathbf{y} = (-3 \ 2 \ 0)^\top$  we have  $\text{supp}(\mathbf{y}) = \{1, 2\}$  and  $\text{supp}_{\geq 0}(\mathbf{y}) = \{2, 3\}$ .

For a symmetric matrix  $\mathbf{X} \in \mathbb{R}^{n \times n}$ , a vector  $\mathbf{v} \in \mathbb{R}^n$  and a set of indices  $\mathcal{I} \in \mathbb{P}[n]$  we define  $\mathbf{X}_{\mathcal{I}} \in \mathcal{S}^{|\mathcal{I}|}$  to be the principal submatrix of  $\mathbf{X}$  corresponding to  $\mathcal{I}$ , and we define  $\mathbf{v}_{\mathcal{I}} \in \mathbb{R}^{|\mathcal{I}|}$  to be the subvector of  $\mathbf{v}$  corresponding to  $\mathcal{I}$ . For simplicity the numbering of the indices is preserved, e.g. for

$$\mathbf{X} = \begin{pmatrix} 1 & 6 & 3 \\ 6 & 9 & 2 \\ 3 & 2 & 8 \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} 4 \\ 0 \\ 7 \end{pmatrix}, \quad \mathcal{I} = \{2, 3\},$$

we have

$$\mathbf{X}_{\mathcal{I}} = \begin{pmatrix} 9 & 2 \\ 2 & 8 \end{pmatrix}, \quad \mathbf{v}_{\mathcal{I}} = \begin{pmatrix} 0 \\ 7 \end{pmatrix},$$

and we say that 0 is the 2nd entry of  $\mathbf{v}_{\mathcal{I}}$  and 2 is the (2, 3) entry of  $\mathbf{X}_{\mathcal{I}}$ .

Note that if  $\mathbf{X} \in \mathcal{S}^n$  and  $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$  and  $\mathcal{I} \in \mathbb{P}[n]$  with  $\text{supp}(\mathbf{u}) \cup \text{supp}(\mathbf{v}) \subseteq \mathcal{I}$  then  $(\mathbf{X}\mathbf{v})_{\mathcal{I}} = \mathbf{X}_{\mathcal{I}}\mathbf{v}_{\mathcal{I}}$  and  $\mathbf{u}^\top \mathbf{X}\mathbf{v} = \mathbf{u}_{\mathcal{I}}^\top (\mathbf{X}\mathbf{v})_{\mathcal{I}} = (\mathbf{X}\mathbf{u})_{\mathcal{I}}^\top \mathbf{v}_{\mathcal{I}} = \mathbf{u}_{\mathcal{I}}^\top \mathbf{X}_{\mathcal{I}}\mathbf{v}_{\mathcal{I}}$ . From this observation we get the well known result that if a matrix is copositive then all its principal submatrices must also be copositive.

Finally, for  $\mathcal{I} \in \mathbb{P}[n]$  and  $\mathbf{u} \in \mathbb{R}^{|\mathcal{I}|}$  (indexed by  $\mathcal{I}$ ) we let  $\mathbf{u}_{-\mathcal{I}} \in \mathbb{R}^n$  be such that

$$(\mathbf{u}_{-\mathcal{I}})_i = \begin{cases} 0 & \text{if } i \notin \mathcal{I} \\ u_i & \text{if } i \in \mathcal{I} \end{cases}.$$

### 3 Certifying Noncopositivity

Given a matrix  $\mathbf{X} \in \mathcal{S}^n \setminus \mathcal{COP}^n$ , a natural certificate that  $\mathbf{X}$  is not copositive would be a vector  $\mathbf{v} \in \mathbb{R}_+^n$  such that  $\mathbf{v}^\top \mathbf{X}\mathbf{v} < 0$ . But how do we find such a vector? This is a major problem in copositivity research and a number of different methods exist for doing this. We will focus on a method derived from the following result.

**Theorem 3.1** ([20, Theorem 2]). *Let  $\mathbf{X} \in \mathcal{S}^n$  such that either  $n = 1$  or  $\mathbf{X}_{[1:n] \setminus \{i\}} \in \mathcal{COP}^{n-1}$  for all  $i \in [1:n]$ . Then  $\mathbf{X} \notin \mathcal{COP}^n$  if and only if  $\mathbf{X}$  is nonsingular with  $-\mathbf{X}^{-1} \in \mathcal{N}^n$ .*

This theorem can be used to prove the following results:

**Lemma 3.2.** *Let  $\mathbf{X} \in \mathcal{S}^n$  such that either  $n = 1$  or  $\mathbf{X}_{[1:n] \setminus \{i\}} \in \mathcal{COP}^{n-1}$  for all  $i \in [1:n]$ . Then the following are equivalent:*

1.  $\mathbf{X} \notin \mathcal{COP}^n$ ;
2.  $\mathbf{X}$  is nonsingular and  $-\mathbf{X}^{-1} \in \mathcal{N}^n$ ;
3.  $\forall \mathbf{b} \in \mathbb{R}_+^n, \exists \mathbf{u} \in \mathbb{R}_+^n$  with  $\mathbf{X}\mathbf{u} = -\mathbf{b}$ ,

4.  $\exists \mathbf{u} \in \mathbb{R}_+^n$  such that  $\mathbf{X}\mathbf{u} = -\mathbf{1}_n$ .

5.  $\exists \mathbf{u} \in \mathbb{R}_+^n$  such that  $-\mathbf{X}\mathbf{u} \in \mathbb{R}_{++}^n$ .

*Proof.* We trivially have  $2 \Rightarrow 3 \Rightarrow 4 \Rightarrow 5$ , and from Theorem 3.1 we have  $1 \Rightarrow 2$ . We complete the proof by noting that if 5 holds then  $\mathbf{u} \in \mathbb{R}_+^n \setminus \{\mathbf{0}_n\}$  and  $\mathbf{u}^\top \mathbf{X}\mathbf{u} = -\mathbf{u}^\top (-\mathbf{X}\mathbf{u}) < 0$ , and thus  $5 \Rightarrow 1$ .  $\square$

**Theorem 3.3.** *For  $\mathbf{X} \in \mathcal{S}^n$  the following are equivalent:*

1.  $\mathbf{X} \notin \mathcal{COP}^n$ ,

2.  $\exists \mathcal{I} \in \mathbb{P}[n]$  and  $\mathbf{u} \in \mathbb{R}_+^{|\mathcal{I}|}$  such that  $\mathbf{X}_{\mathcal{I}}\mathbf{u} = -\mathbf{1}_{|\mathcal{I}|}$ .

3.  $\exists \mathcal{I} \in \mathbb{P}[n]$  and  $\mathbf{u} \in \mathbb{R}_+^{|\mathcal{I}|}$  such that  $-\mathbf{X}_{\mathcal{I}}\mathbf{u} \in \mathbb{R}_{++}^{|\mathcal{I}|}$ .

This means that we can check whether a matrix  $\mathbf{X}$  is copositive by going through all the principal submatrices  $\mathbf{X}_{\mathcal{I}}$  of it and attempting to solve  $\mathbf{X}_{\mathcal{I}}\mathbf{u} = -\mathbf{1}_{|\mathcal{I}|}$ . Note that we do not in fact need to solve  $\mathbf{X}_{\mathcal{I}}\mathbf{u} = -\mathbf{1}_{|\mathcal{I}|}$  exactly as it is sufficient to find a solution to  $-\mathbf{X}_{\mathcal{I}}\mathbf{u} \in \mathbb{R}_{++}^{|\mathcal{I}|}$ , or to establish that  $\mathbf{X}_{\mathcal{I}}$  is singular.

The problem with this method is that there are exponentially many principal submatrices to check, as  $|\mathbb{P}[n]| = 2^n - 1$ . However for each principal submatrix we need only solve a linear system, making it simpler than an alternative well known method of checking the eigenvectors and eigenvalues of all the principal submatrices, as introduced in [27] and recalled below:

**Theorem 3.4** ([27, Theorem 2]). *For  $\mathbf{X} \in \mathcal{S}^n$  we have that  $\mathbf{X} \notin \mathcal{COP}^n$  if and only if  $\exists \mathcal{I} \in \mathbb{P}[n]$  with an eigenvector  $\mathbf{v} \in \mathbb{R}_+^{|\mathcal{I}|}$  and corresponding eigenvalue  $\lambda < 0$ .*

Another problem with the method introduced in this section is that if a matrix is copositive, then no simple certificate for this is produced. We shall discuss this further in the following section.

## 4 Certifying Copositivity

In this section, we will present a new method for certifying a matrix to be copositive. This new certificate will be derived from Theorem 3.3, and in order to do this, we first need to recall the well known Farkas' lemma. In this lemma and the subsequent results we say that two systems are alternative systems if exactly one of them must hold (e.g. for  $x \in \mathbb{R}$ , the systems " $x > 0$ " and " $x \leq 0$ " would be alternative systems).

**Lemma 4.1** ([19]). *For  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and  $\mathbf{b} \in \mathbb{R}^m$  the following are alternative systems:*

1.  $\exists \mathbf{x} \in \mathbb{R}_+^n$  such that  $\mathbf{A}\mathbf{x} = \mathbf{b}$ ,

2.  $\exists \mathbf{y} \in \mathbb{R}^m$  such that  $\mathbf{A}^\top \mathbf{y} \in \mathbb{R}_+^n$  and  $\mathbf{b}^\top \mathbf{y} < 0$ .

We will need the following two corollaries of this result.

**Corollary 4.2.** *For  $\mathbf{X} \in \mathcal{S}^n$  and  $\mathbf{b} \in \mathbb{R}^n$  the following are alternative systems:*

1.  $\exists \mathbf{u} \in \mathbb{R}_+^n$  such that  $\mathbf{X}\mathbf{u} = -\mathbf{b}$ ,

2.  $\exists \mathbf{w} \in \mathbb{R}^n$  such that  $\mathbf{X}\mathbf{w} \in \mathbb{R}_+^n$  and  $\mathbf{b}^\top \mathbf{w} = 1$ .

*Proof.* From Lemma 4.1 we have that an alternative statement to statement 1 of this corollary is that  $\exists \mathbf{y} \in \mathbb{R}^n$  such that  $\mathbf{X}^\top \mathbf{y} \in \mathbb{R}_+^m$  and  $(-\mathbf{b})^\top \mathbf{y} < 0$ , which is equivalent to statement 2 of this corollary.  $\square$

**Corollary 4.3.** For  $\mathbf{X} \in \mathcal{S}^n$  the following are alternative systems:

1.  $\exists \mathbf{u} \in \mathbb{R}_+^n$  such that  $-\mathbf{X}\mathbf{u} \in \mathbb{R}_{++}^n$ ,
2.  $\exists \mathbf{z} \in \mathbb{R}_+^n \setminus \{\mathbf{0}_n\}$  such that  $\mathbf{X}\mathbf{z} \in \mathbb{R}_+^n$ .

*Proof.* These statements are equivalent respectively to the following two statements, which by Lemma 4.1 are alternative systems:

1.  $\exists \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \in \mathbb{R}_+^{2n}$  such that  $\begin{pmatrix} \mathbf{X} & \mathbf{I}_n \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = -\mathbf{1}_n$ ,
2.  $\exists \mathbf{z} \in \mathbb{R}^n$  such that  $\begin{pmatrix} \mathbf{X} \\ \mathbf{I}_n \end{pmatrix} \mathbf{z} \in \mathbb{R}_+^{2n}$  and  $(-\mathbf{1}_n)^\top \mathbf{z} < 0$ .  $\square$

By considering the alternative systems for the statements in Lemma 3.2 and then simplifying, we now get the following results:

**Lemma 4.4.** Let  $\mathbf{X} \in \mathcal{S}^n$  such that either  $n = 1$  or  $\mathbf{X}_{[1:n] \setminus \{i\}} \in \mathcal{COP}^{n-1}$  for all  $i \in [1:n]$ . Then the following are equivalent:

1.  $\mathbf{X} \in \mathcal{COP}^n$ ,
2. Either  $\mathbf{X}$  is singular or  $\mathbf{X}$  is nonsingular and  $-\mathbf{X}^{-1} \notin \mathcal{N}^n$ ,
3.  $\exists \mathbf{y} \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$ <sup>2</sup> such that  $\mathbf{X}\mathbf{y} \in \mathbb{R}_+^n$ ,
4.  $\exists \mathbf{y} \in \mathbb{R}^n$  such that  $\mathbf{X}\mathbf{y} \in \mathbb{R}_+^n$  and  $\mathbf{1}_n^\top \mathbf{y} = 1$ ,
5.  $\exists \mathbf{y} \in \mathbb{R}_+^n \setminus \{\mathbf{0}_n\}$  such that  $\mathbf{X}\mathbf{y} \in \mathbb{R}_+^n$ .

*Proof.* It is trivial to see that 1 and 2 make alternative systems with their corresponding statements in Lemma 3.2.

We will now show that 3 also makes an alternative system with its corresponding statement in Lemma 3.2. To do this, we show that the following statements are equivalent:

- (a)  $\neg (\forall \mathbf{b} \in \mathbb{R}_+^n, \exists \mathbf{u} \in \mathbb{R}_+^n \text{ with } \mathbf{X}\mathbf{u} = -\mathbf{b})$ ;
- (b)  $\exists \mathbf{b} \in \mathbb{R}_+^n, \neg (\exists \mathbf{u} \in \mathbb{R}_+^n \text{ with } \mathbf{X}\mathbf{u} = -\mathbf{b})$ ;
- (c)  $\exists \mathbf{b} \in \mathbb{R}_+^n, \exists \mathbf{y} \in \mathbb{R}^n \text{ with } \mathbf{X}\mathbf{y} \in \mathbb{R}_+^n \text{ and } \mathbf{b}^\top \mathbf{y} = 1$ ;
- (d)  $\exists \mathbf{y} \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  such that  $\mathbf{X}\mathbf{y} \in \mathbb{R}_+^n$ .

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<sup>2</sup>In other words  $\mathbf{y} \in \mathbb{R}^n$  has at least one strictly positive entry.

Trivially (a) and (b) are equivalent, and the equivalence of (b) and (c) follows from Corollary 4.2.

If (c) holds then trivially (d) holds.

Conversely, if (d) holds then there exists  $i \in [1:n]$  such that  $y_i > 0$ , and letting  $\mathbf{b} = \frac{1}{y_i} \mathbf{e}_i \in \mathbb{R}_+^n$  we get  $\mathbf{b}^\top \mathbf{y} = 1$ , and thus (c) holds.

A similar proof, using Corollaries 4.2 and 4.3, can be used to show that 4 and 5 also make alternative systems with their corresponding statements in Lemma 3.2.  $\square$

*example 4.5.* Consider the so-called Horn matrix, which was originally constructed by Prof. Alfred Horn [9]:

$$\mathbf{H} = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}.$$

This has been shown to be copositive using multiple methods (e.g. [4, 6, 8, 22, 33, 36]), and we now add yet another method to the mix.

For all  $i \in [1:5]$  we have that  $\mathbf{H}_{[1:5] \setminus \{i\}}$  is equivalent after permutations to

$$\mathbf{H}_{[1:4]} = (\mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_3 - \mathbf{e}_4)(\mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_3 - \mathbf{e}_4)^\top + 2(\mathbf{e}_1 \mathbf{e}_4^\top + \mathbf{e}_4 \mathbf{e}_1^\top) \in \mathcal{SPN}^4 = \mathcal{COP}^4.$$

We also have  $\mathbf{H}\mathbf{1}_5 = \mathbf{1}_5 \in \mathbb{R}_+^5$ , and thus by Lemma 4.4 we have  $\mathbf{H} \in \mathcal{COP}^5$ .

Now, we are ready to present the main result of this paper, which follows from Lemma 4.4.

**Theorem 4.6.** *For  $\mathbf{X} \in \mathcal{S}^n$  we have that  $\mathbf{X} \in \mathcal{COP}^n$  if and only if there exists  $\mathcal{U} \subseteq \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  such that  $\forall \mathcal{I} \in \mathbb{P}[n]$ ,  $\exists \mathbf{u} \in \mathcal{U}$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ .*

*Proof.* We will first show that if  $\mathbf{X}$  is copositive then such a set  $\mathcal{U}$  must exist. Considering an arbitrary  $\mathcal{I} \in \mathbb{P}[n]$ , by Lemma 4.4, there exists  $\mathbf{y} \in \mathbb{R}^{|\mathcal{I}|} \setminus (-\mathbb{R}_+^{|\mathcal{I}|})$  such that  $\mathbf{X}_{\mathcal{I}}\mathbf{y} \in \mathbb{R}_+^{|\mathcal{I}|}$ . Letting  $\mathbf{u} = \mathbf{y}_{-\mathcal{I}}$ , we then have  $\mathbf{u} \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I}$  and  $(\mathbf{X}\mathbf{u})_{\mathcal{I}} = \mathbf{X}_{\mathcal{I}}\mathbf{y} \in \mathbb{R}_+^{|\mathcal{I}|}$ .

We will now complete the proof by showing that if  $\mathbf{X}$  is not copositive then such a set  $\mathcal{U}$  can not exist. Suppose for the sake of contradiction that  $\mathbf{X} \notin \mathcal{COP}^n$  but such a set  $\mathcal{U}$  does exist. As  $\mathbf{X} \notin \mathcal{COP}^n$ , there exists  $\mathcal{I} \in \mathbb{P}[n]$  such that  $\mathbf{X}_{\mathcal{I}} \notin \mathcal{COP}^{|\mathcal{I}|}$  and either  $|\mathcal{I}| = 1$  or  $\mathbf{X}_{\mathcal{I} \setminus \{i\}} \in \mathcal{COP}^{|\mathcal{I}|-1}$  for all  $i \in \mathcal{I}$ . From the requirements on  $\mathcal{U}$ , there exists  $\mathbf{u} \in \mathcal{U} \subseteq \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ . Letting  $\mathbf{y} = \mathbf{u}_{\mathcal{I}}$  we then have  $\mathbf{y} \in \mathbb{R}^{|\mathcal{I}|} \setminus (-\mathbb{R}_+^{|\mathcal{I}|})$  and  $\mathbf{X}_{\mathcal{I}}\mathbf{y} = (\mathbf{X}\mathbf{u})_{\mathcal{I}} \in \mathbb{R}_+^{|\mathcal{I}|}$ . By Lemma 4.4 this then gives the contradiction that  $\mathbf{X}_{\mathcal{I}} \in \mathcal{COP}^{|\mathcal{I}|}$ .  $\square$

*Remark 4.7.* Note that by Lemma 4.4, in Theorem 4.6 we could have in fact had the more restrictive requirement that  $\mathcal{U} \subseteq \mathbb{R}_+^n \setminus \{\mathbf{0}_n\}$ , and for all of the examples in this paper we do indeed have that  $\mathcal{U} \subseteq \mathbb{R}_+^n \setminus \{\mathbf{0}_n\}$ . We have however decided to leave the Theorem in its more general form.

*example 4.8.* Consider the matrix

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

From [25, 37] we have that  $\mathbf{X} \in \mathcal{COP}^5 \setminus \mathcal{SPN}^5$ . We can certify that this matrix is copositive by considering the following  $\mathcal{U}$ , which conforms to the requirements of Theorem 4.6:  $\mathcal{U} = \{ \mathbf{e}_i : i \in [1:5] \} \cup \{ \mathbf{e}_i + \mathbf{e}_{i+1} : i \in [1:4] \}$ . This is shown in Table 1, where for all  $\mathcal{I} \in \mathbb{P}[5]$  we give a  $\mathbf{u} \in \mathcal{U}$  such that  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ .

$\mathcal{I}$	$\mathbf{u}$	$\mathcal{I}$	$\mathbf{u}$	$\mathcal{I}$	$\mathbf{u}$	$\mathcal{I}$	$\mathbf{u}$
{1}	$\mathbf{e}_1$	{1, 5}	$\mathbf{e}_1$	{1, 2, 4}	$\mathbf{e}_4$	{3, 4, 5}	$\mathbf{e}_3 + \mathbf{e}_4$
{2}	$\mathbf{e}_2$	{2, 3}	$\mathbf{e}_2 + \mathbf{e}_3$	{1, 2, 5}	$\mathbf{e}_5$	{1, 2, 3, 4}	$\mathbf{e}_1 + \mathbf{e}_2$
{3}	$\mathbf{e}_3$	{2, 4}	$\mathbf{e}_2$	{1, 3, 4}	$\mathbf{e}_1$	{1, 2, 3, 5}	$\mathbf{e}_1 + \mathbf{e}_2$
{4}	$\mathbf{e}_4$	{2, 5}	$\mathbf{e}_2$	{1, 3, 5}	$\mathbf{e}_1$	{1, 2, 4, 5}	$\mathbf{e}_1 + \mathbf{e}_2$
{5}	$\mathbf{e}_5$	{3, 4}	$\mathbf{e}_3 + \mathbf{e}_4$	{1, 4, 5}	$\mathbf{e}_1$	{1, 3, 4, 5}	$\mathbf{e}_3 + \mathbf{e}_4$
{1, 2}	$\mathbf{e}_1 + \mathbf{e}_2$	{3, 5}	$\mathbf{e}_3$	{2, 3, 4}	$\mathbf{e}_2 + \mathbf{e}_3$	{2, 3, 4, 5}	$\mathbf{e}_2 + \mathbf{e}_3$
{1, 3}	$\mathbf{e}_1$	{4, 5}	$\mathbf{e}_4 + \mathbf{e}_5$	{2, 3, 5}	$\mathbf{e}_5$	{1, 2, 3, 4, 5}	$\mathbf{e}_1 + \mathbf{e}_2$
{1, 4}	$\mathbf{e}_1$	{1, 2, 3}	$\mathbf{e}_1 + \mathbf{e}_2$	{2, 4, 5}	$\mathbf{e}_2$		

Table 1: Enumerating how  $\mathcal{U}$  certifies  $\mathbf{X}$  to be copositive in Example 4.8.

A basic sketch of how to find such a certificate is provided by Algorithms 1 and 2.

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**Algorithm 1** Generating certificates to confirm whether a matrix is copositive or not.

---

**Input:**  $\mathbf{X} \in \mathcal{S}^n$ .

**Output:** Either:

- i.  $\mathbf{v} \in \mathbb{R}_+^n$  such that  $\mathbf{v}^\top \mathbf{X} \mathbf{v} < 0$  (certifying that  $\mathbf{X} \notin \mathcal{COP}^n$ ), or
- ii.  $\mathcal{U} \subseteq \mathbb{R}^n$  such that  $\mathbf{X}$  and  $\mathcal{U}$  conform to the requirements of Theorem 4.6 (certifying that  $\mathbf{X} \in \mathcal{COP}^n$ ).

- 1:  $\mathcal{U} := \emptyset$ .
  - 2: **for**  $\mathcal{I} \in \mathbb{P}[n]$  s. t.  $\nexists \mathbf{u} \in \mathcal{U}$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$  **do**
  - 3:   Input  $\mathbf{X}_{\mathcal{I}}$  into Algorithm 2 and let  $\mathbf{w} \in \mathbb{R}^{|\mathcal{I}|}$  be the output.
  - 4:   **if**  $-\mathbf{w} \in \mathbb{R}_+^{|\mathcal{I}|}$  **then**
  - 5:     Output  $\mathbf{v} = -\mathbf{w}_{-\mathcal{I}} \in \mathbb{R}_+^n$  and **exit**.
  - 6:   **else**
  - 7:     Let  $\mathbf{u} = \mathbf{w}_{-\mathcal{I}} \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  and let  $\mathcal{U} \leftarrow \mathcal{U} \cup \{\mathbf{u}\}$ .
  - 8:   **end if**
  - 9: **end for**
- 

---

**Algorithm 2** Generating vectors necessary in checking copositivity through (approximately) solving linear systems

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**Input:**  $\mathbf{X} \in \mathcal{S}^m$ .

**Output:**  $\mathbf{w} \in \mathbb{R}^m$  such that  $\mathbf{X}\mathbf{w} \in \mathbb{R}_{++}^m \cup \{\mathbf{0}_m\}$  and  $(\mathbf{X}\mathbf{w}, -\mathbf{w}) \notin \{\mathbf{0}_m\} \times \mathbb{R}_+^m$ .

- 1: Attempt to (approximately) solve  $\mathbf{X}\mathbf{w} = \mathbf{1}_m$  to find  $\mathbf{w} \in \mathbb{R}^m$  s. t.  $\mathbf{X}\mathbf{w} \in \mathbb{R}_{++}^m$ .
  - 2: **If** unable to (approximately) solve  $\mathbf{X}\mathbf{w} = \mathbf{1}_m$ , as  $\mathbf{X}$  is singular, **then** find a  $\mathbf{w} \in \mathbb{R}^m \setminus (-\mathbb{R}_+^m)$  in the null space of  $\mathbf{X}$ .
- 

If Algorithm 1 ends at a step 5 then we have  $\mathbf{v} \in \mathbb{R}_+^n$  and  $\mathbf{v}^\top \mathbf{X} \mathbf{v} = \mathbf{w}^\top \mathbf{X}_{\mathcal{I}} \mathbf{w} < 0$ , and thus the algorithm stops with output i..

If Algorithm 1 never ends at a step 5, then for each  $\mathcal{I}$  considered, step 7 is carried out. In this case we add to  $\mathcal{U}$  a vector  $\mathbf{u} \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  such that  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I}$

and  $(\mathbf{X}\mathbf{u})_{\mathcal{I}} = \mathbf{X}_{\mathcal{I}}\mathbf{w} \in \mathbb{R}_{++}^{|\mathcal{I}|} \cup \{\mathbf{0}_{|\mathcal{I}|}\}$ . Therefore, upon completion of the algorithm, we have a set  $\mathcal{U} \subseteq \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  such that for all  $\mathcal{I} \in \mathbb{P}[n]$  there exists a  $\mathbf{u} \in \mathcal{U}$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ , and thus the algorithm stops with output ii..

We thus see that the algorithm will complete in finite time, and for whichever conclusion the algorithm reaches (copositive or not) there is a certificate to confirm this result. We also note that throughout the algorithm we only need to solve linear systems, and thus the individual steps of the algorithm are relatively simple.

Note that in step 1 of Algorithm 2, we can replace  $\mathbf{1}_m$  with any vector in  $\mathbb{R}_{++}^m$  and the algorithm would still complete as before, although with a different vector  $\mathbf{w} \in \mathbb{R}^m$ . In fact from this observation we see that this algorithm allows for small numerical errors, as we try to solve  $\mathbf{X}_{\mathcal{I}}\mathbf{w} = \mathbf{1}_{|\mathcal{I}|}$ , but only require  $\mathbf{X}_{\mathcal{I}}\mathbf{w} \in \mathbb{R}_{++}^{|\mathcal{I}|}$ .

A final advantage of Algorithm 1 is that although we still have to deal with lots of principal submatrices, we do not necessarily have to solve a linear system for each of them. This is demonstrated by reconsidering Example 4.8, where we see that producing this certificate would not require solving any linear systems corresponding to  $|\mathcal{I}| \geq 3$ . The main difficulty in implementing this algorithm would be to find an efficient way to go through the principal submatrices.

We finish this section by observing that using our new method even copositive matrices which are not in  $\mathcal{SPN}^n$  may have very small certificates of copositivity. In Example 4.8 we considered a matrix of order five which was copositive but not positive semidefinite plus nonnegative whose certificate was of cardinality 9 (in comparison to  $|\mathbb{P}[5]| = 2^5 - 1 = 31$ ). We now consider a more general set of examples as an extension of the results from [25, 37].

**Lemma 4.9.** *Consider  $\mathbf{X} \in \mathcal{S}^n$  such that  $x_{ii} = 1$  and  $x_{ij} \in \{-1\} \cup \mathbb{R}_+$  for all  $i, j$ , and let  $G$  be a graph on  $n$  vertices with an edge between vertices  $i, j$  if and only if  $x_{ij} = -1$ . Then we have*

1.  $\mathbf{X} \in \mathcal{SPN}^n$  if and only if  $G$  is bipartite and  $x_{ij} \geq 1$  whenever there is an even length path between  $i$  and  $j$  in  $G$ .
2.  $\mathbf{X} \in \mathcal{COP}^n$  if and only if  $x_{ij} \geq 1$  whenever there is a path of length 2 between  $i$  and  $j$  in  $G$  (and thus  $G$  is triangle free). Furthermore, a certificate certifying such matrices to be copositive with cardinality at most  $n + \lfloor n^2/4 \rfloor$  is given by

$$\mathcal{U} = \{\mathbf{e}_i : i \in [1:n]\} \cup \{\mathbf{e}_i + \mathbf{e}_j : x_{ij} = -1, i < j\}.$$

*Proof.* The condition for  $\mathbf{X} \in \mathcal{SPN}^n$  comes directly from [37, Lemma 3.5].

We now consider the condition for  $\mathbf{X} \in \mathcal{COP}^n$ . From Mantel's theorem [29] we have that if  $G$  is triangle free then it has at most  $\lfloor n^2/4 \rfloor$  edges, and thus  $|\mathcal{U}| \leq n + \lfloor n^2/4 \rfloor$ . We will now complete the proof by showing that the following statements are equivalent for  $\mathbf{X}$  as given in the lemma:

- (a)  $\mathbf{X} \in \mathcal{COP}^n$ ;
- (b)  $x_{ij} \geq 1$  whenever  $x_{ik} = x_{jk} = -1$  for some  $k$ ;
- (c) For  $\mathcal{U}$  as given have  $\forall \mathcal{I} \in \mathbb{P}[n], \exists \mathbf{u} \in \mathcal{U}$  such that  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ .

As  $\mathcal{U} \subseteq \mathbb{R}_+^n$ , from Theorem 4.6 we have that statement (c) implies statement (a).

To show that statement (a) implies statement (b) we assume for the sake of contradiction that  $\mathbf{X} \in \mathcal{COP}^n$  and  $\exists i, j, k$  such that  $x_{ij} < 1 = -x_{ik} = -x_{jk}$ . Then for  $\mathbf{v} = (\mathbf{e}_i + \mathbf{e}_j + 2\mathbf{e}_k) \in \mathbb{R}_+^n$  we get the contradiction  $\mathbf{v}^T \mathbf{X} \mathbf{v} = 2(x_{ij} - 1) < 0$ .



We are now left to show that statement (b) implies statement (c). Consider an arbitrary  $\mathcal{I} \in \mathbb{P}[n]$ .

If  $x_{ij} \geq 0$  for all  $i, j \in \mathcal{I}$ , then for arbitrary  $i \in \mathcal{I}$  letting  $\mathbf{u} = \mathbf{e}_i \in \mathcal{U}$  we have  $\text{supp}(\mathbf{u}) = \{i\} \subseteq \mathcal{I}$  and  $\mathcal{I} \subseteq \{j : x_{ij} \geq 0\} = \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ .

If on the other hand  $x_{ij} = -1$  for some  $i, j \in \mathcal{I}$ , then letting  $\mathbf{u} := (\mathbf{e}_i + \mathbf{e}_j) \in \mathcal{U}$  we have  $\text{supp}(\mathbf{u}) = \{i, j\} \subseteq \mathcal{I}$ . For  $k \in [1:n]$ , if  $-1 \in \{x_{ik}, x_{jk}\}$  then by statement (b) we have  $\max\{x_{ik}, x_{jk}\} \geq 1$  and  $x_{ik} + x_{jk} \geq 0$ . Alternatively, if  $-1 \notin \{x_{ik}, x_{jk}\}$  then  $x_{ik}, x_{jk} \geq 0$  and  $x_{ik} + x_{jk} \geq 0$ . Therefore  $(\mathbf{X}\mathbf{u})_k = x_{ik} + x_{jk} \geq 0$  for all  $k \in [1:n]$  and  $\mathcal{I} \subseteq [1:n] = \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ .  $\square$

We thus have a set of matrices which are copositive but not positive semidefinite plus nonnegative, whose certificates of copositivity grow at most quadratically with  $n$  (whilst  $|\mathbb{P}[n]| = 2^n - 1$  grows exponentially). From [22, 25] this includes some extremal copositive matrices which are not positive semidefinite plus nonnegative.

In Lemma 5.2 we will see that the certificate  $\mathcal{U}$  given in Lemma 4.9 is in fact a certificate of minimal cardinality.

## 5 Minimal Zeros

In this short section we will briefly look at how this new certificate is related to the so-called set of zeros of a matrix [9, 23].

**Definition 5.1.** For  $\mathbf{X} \in \mathcal{COP}^n$  we define its *set of zeros*,  $\mathcal{V}^{\mathbf{X}} := \{\mathbf{u} \in \mathbb{R}_+^n \setminus \{\mathbf{0}_n\} : \mathbf{u}^\top \mathbf{X} \mathbf{u} = 0\}$ , and its *set of minimal zeros*,  $\mathcal{V}_{\min}^{\mathbf{X}} := \{\mathbf{v} \in \mathcal{V}^{\mathbf{X}} : \nexists \mathbf{u} \in \mathcal{V}^{\mathbf{X}} \text{ s. t. } \text{supp}(\mathbf{u}) \subsetneq \text{supp}(\mathbf{v})\}$ .

In [23] it was shown that for a copositive matrix the set of minimal zeros is always a finite set (up to multiplication by a positive scalar). We will now see that  $\mathcal{V}_{\min}^{\mathbf{X}}$  is also contained in a certificate of copositivity for it.

**Lemma 5.2.** *Let  $\mathbf{X} \in \mathcal{COP}^n$  and  $\mathcal{U} \subseteq \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  such that  $\forall \mathcal{I} \in \mathbb{P}[n], \exists \mathbf{u} \in \mathcal{U}$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ . Then for all  $\mathbf{v} \in \mathcal{V}_{\min}^{\mathbf{X}}$  we have  $\lambda \mathbf{v} \in \mathcal{U}$  for some  $\lambda > 0$ .*

*Proof.* Consider an arbitrary  $\mathbf{v} \in \mathcal{V}_{\min}^{\mathbf{X}}$  and let  $\mathcal{I} = \text{supp}(\mathbf{v})$ . There exists  $\mathbf{u} \in \mathcal{U}$  such that  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ . From [13, Lemma 2.5] we have  $(\mathbf{X}\mathbf{v})_{\mathcal{I}} = \mathbf{0}_{|\mathcal{I}|}$  and thus  $0 = \mathbf{u}_{\mathcal{I}}^\top \mathbf{0}_{|\mathcal{I}|} = \mathbf{u}_{\mathcal{I}}^\top (\mathbf{X}\mathbf{v})_{\mathcal{I}} = \mathbf{u}_{\mathcal{I}}^\top \mathbf{X}\mathbf{v} = \mathbf{v}_{\mathcal{I}}^\top (\mathbf{X}\mathbf{u})_{\mathcal{I}}$ . As  $\mathbf{v}_{\mathcal{I}} \in \mathbb{R}_{++}^{|\mathcal{I}|}$  and  $(\mathbf{X}\mathbf{u})_{\mathcal{I}} \in \mathbb{R}_+^{|\mathcal{I}|}$ , this implies that  $\mathbf{0}_{|\mathcal{I}|} = (\mathbf{X}\mathbf{u})_{\mathcal{I}} = \mathbf{X}_{\mathcal{I}} \mathbf{u}_{\mathcal{I}}$ . From [23, Lemma 3.7] we then have that there exists  $\lambda \in \mathbb{R}$  such that  $\mathbf{u}_{\mathcal{I}} = \lambda \mathbf{v}_{\mathcal{I}}$ . Noting that  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} = \text{supp}(\mathbf{v})$ ,  $\mathbf{u} \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  and  $\mathbf{v} \in \mathbb{R}_+^n$  we get that  $\mathbf{u} = \lambda \mathbf{v}$  with  $\lambda > 0$ , completing the proof.  $\square$

Applying this result to Lemma 4.9, it can be seen that the certificate  $\mathcal{U}$  given in this example is the smallest possible (by cardinality).

This lemma is useful in two further ways. Firstly it means that if we find such a certificate as introduced in this paper for a matrix to be copositive then we will get the complete set of minimal zeros for free, as shown in the corollary below. The set of minimal zeros is useful in analysing the matrix, for example when considering the facial structure of the copositive cone [15].

**Corollary 5.3.** *Let  $\mathbf{X} \in \mathcal{COP}^n$  and  $\mathcal{U} \subseteq \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  such that  $\forall \mathcal{I} \in \mathbb{P}[n], \exists \mathbf{u} \in \mathcal{U}$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ . Now let  $\widehat{\mathcal{V}} = \{\mu \mathbf{u} : \mathbf{u} \in \mathcal{U} \cap \mathbb{R}_+^n, \mu \in \mathbb{R}_{++}, \mathbf{u}^\top \mathbf{X} \mathbf{u} = 0\}$ . Then  $\mathcal{V}_{\min}^{\mathbf{X}} \subseteq \widehat{\mathcal{V}} \subseteq \mathcal{V}^{\mathbf{X}}$  and  $\mathcal{V}_{\min}^{\mathbf{X}} = \{\mathbf{u} \in \widehat{\mathcal{V}} : \nexists \mathbf{w} \in \widehat{\mathcal{V}} \text{ with } \text{supp}(\mathbf{w}) \subsetneq \text{supp}(\mathbf{u})\}$ .*

Another advantage is that for a (minimal) zero  $\mathbf{u}$  of  $\mathbf{X}$  we have  $\text{supp}_{\geq 0}(\mathbf{X}\mathbf{u}) = [1:n]$  and thus all sets  $\mathcal{I} \in \mathbb{P}[n]$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I}$  are covered by  $\text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$  when forming the certificates.

## 6 Negative Off-diagonal Entries

In this section we will focus on matrices in  $\mathcal{S}^n$  whose off-diagonal entries are all nonpositive. Such matrices are referred to in the literature as symmetric Z-matrices, whilst such matrices which are copositive are referred to as symmetric M-matrices [2, 35]. We will see that considering such matrices provides both a problem to our current certificates and an extension to them.

For  $\mathbf{A} \in \mathcal{S}^n$  we will define  $G_{\mathbf{A}}$  to be the simple graph on the vertices  $[1:n]$  such that there is an edge between distinct vertices  $i, j$  if and only if  $a_{ij} \neq 0$ . We then have the following results, the first two of which are well known, with proofs being included in Appendix A for the sake of completeness:

**Lemma 6.1.** *Let  $\mathbf{A} \in \mathcal{S}^n$  be a Z-matrix with  $G_{\mathbf{A}}$  is connected. Then  $\mathbf{A}$  has an eigenvector  $\mathbf{v} \in \mathbb{R}_{++}^n$  whose corresponding eigenvalue  $\lambda$  is of geometric multiplicity one and is strictly less than all other eigenvalues of  $\mathbf{A}$ . We then have  $\mathbf{A} \in \text{COP}^n$  if and only if  $\lambda \geq 0$ .*

**Lemma 6.2.** *For a Z-matrix  $\mathbf{A} \in \mathcal{S}^n$  the following are equivalent:*

1.  $\mathbf{A}$  is copositive;
2.  $\mathbf{A}$  is positive semidefinite;
3.  $\exists \mathbf{x} \in \mathbb{R}_{++}^n$  such that  $\mathbf{A}\mathbf{x} \in \mathbb{R}_+^n$ .

**Lemma 6.3.** *For a Z-matrix  $\mathbf{A} \in \mathcal{S}^n$  such that  $G_{\mathbf{A}}$  is connected, let  $\mathbf{u} \in \mathbb{R}^n$  be such that  $\mathbf{A}\mathbf{u} \in \mathbb{R}_+^n$  and  $(\mathbf{A}\mathbf{u}, -\mathbf{u}) \notin \{0_n\} \times \mathbb{R}_+^n$ . Then  $\mathbf{u} \notin \mathbb{R}_+^n \setminus \mathbb{R}_{++}^n$  and*

1.  $\mathbf{A} \in \text{COP}^n$  if and only if  $\mathbf{u} \in \mathbb{R}_{++}^n$ ;
2. If  $\mathbf{A}\mathbf{u} \in \mathbb{R}_{++}^n$  and  $\mathbf{u} \in \mathbb{R}^n \setminus \mathbb{R}_+^n$ , then letting  $\mathbf{y} \in \mathbb{R}_+^n$  such that  $y_j = \max\{0, -u_j\}$  for all  $j \in [1:n]$ , we have  $\mathbf{y}^T \mathbf{A}\mathbf{y} < 0$ .

*Proof.* We consider four cases:

1.  $\mathbf{u} \in \mathbb{R}_+^n \setminus \mathbb{R}_{++}^n$ : From the requirements on  $\mathbf{u}$  we have  $\mathbf{u} \neq \mathbf{0}_n$ , and thus, as  $G_{\mathbf{A}}$  is connected,  $\exists i, j \in [1:n]$  such that  $u_i = 0 < u_j$  and  $a_{ij} < 0$ . We then get the following contradiction, implying that this case cannot occur:

$$0 \leq (\mathbf{A}\mathbf{u})_i = \sum_{k \in \text{supp}(\mathbf{u})} \underbrace{a_{ik}}_{\leq 0} \underbrace{u_k}_{> 0} \leq \underbrace{a_{ij}}_{< 0} \underbrace{u_j}_{> 0} < 0.$$

2.  $\mathbf{u} \in \mathbb{R}_{++}^n$ : Then by Lemma 6.2 we have  $\mathbf{A} \in \text{COP}^n$ .
3.  $\mathbf{u} \in \mathbb{R}^n \setminus \mathbb{R}_+^n$  and  $\mathbf{A}\mathbf{u} = \mathbf{0}_n$ : Then by the assumptions we additionally have  $-\mathbf{u} \notin \mathbb{R}_+^n$ . We then have that  $\mathbf{u}$  is an eigenvector of  $\mathbf{A}$  with corresponding eigenvalue equal to zero. By Lemma 6.1, there exists another eigenvalue of  $\mathbf{A}$  which is strictly negative and  $\mathbf{A} \notin \text{COP}^n$ .

4.  $\mathbf{u} \in \mathbb{R}^n \setminus \mathbb{R}_+^n$  and  $\mathbf{A}\mathbf{u} \in \mathbb{R}_+^n \setminus \{\mathbf{0}_n\}$ : If  $\mathbf{A}$  is nonsingular, then from the results of [2, Chapter 6], in particular case (N<sub>39</sub>), we have that  $\mathbf{A} \notin \mathcal{PSD}^n$ , and thus by Lemma 6.2 we have  $\mathbf{A} \notin \mathcal{COP}^n$ . Conversely, if  $\mathbf{A}$  is singular, suppose for the sake of contradiction that  $\mathbf{A} \in \mathcal{COP}^n$ . Then by Lemma 6.1, there exists  $\mathbf{v} \in \mathbb{R}_{++}^n$  such that  $\mathbf{A}\mathbf{v} = \mathbf{0}_n$  and we have the contradiction  $0 < \mathbf{v}^\top(\mathbf{A}\mathbf{u}) = \mathbf{u}^\top(\mathbf{A}\mathbf{v}) = 0$ .

We now complete the proof by supposing that  $\mathbf{A}\mathbf{u} \in \mathbb{R}_{+++}^n$  and  $\mathbf{u} \in \mathbb{R}^n \setminus \mathbb{R}_+^n$ . Letting  $\mathcal{I} = \text{supp}_{\geq 0}(\mathbf{u})$ ,  $\mathcal{J} = [1:n] \setminus \mathcal{I} \neq \emptyset$  and  $\mathbf{y} = (-\mathbf{u}_{\mathcal{J}})_{-\mathcal{J}} \in \mathbb{R}_+^n$ , we have

$$\mathbf{y}^\top \mathbf{A}\mathbf{y} = -\mathbf{y}^\top \mathbf{A}\mathbf{u} + \mathbf{y}^\top \mathbf{A}(\mathbf{u} + \mathbf{y}) = - \underbrace{\mathbf{y}_{\mathcal{J}}^\top}_{\in \mathbb{R}_{++}^{|\mathcal{J}|}} \underbrace{(\mathbf{A}\mathbf{u})_{\mathcal{J}}}_{\in \mathbb{R}_{++}^{|\mathcal{J}|}} - \underbrace{\mathbf{u}_{\mathcal{I}}^\top}_{\in \mathbb{R}_+^{|\mathcal{I}|}} \underbrace{(-\mathbf{A}\mathbf{y})_{\mathcal{I}}}_{\in \mathbb{R}_+^{|\mathcal{I}|}} < 0. \quad \square$$

**Corollary 6.4.** *Consider a Z-matrix  $\mathbf{A} \in \mathcal{COP}^n$  and let  $\mathcal{U}$  be as in Theorem 4.6. Then for all  $\mathbf{u} \in \mathcal{U}$  with  $\text{supp}(\mathbf{u}) \subseteq \text{supp}_{\geq 0}(\mathbf{A}\mathbf{u})$  we have  $\text{supp}(\mathbf{u}) = \text{supp}_{\geq 0}(\mathbf{A}\mathbf{u})$ , and thus  $|\mathcal{U}| \geq |\mathbb{P}[n]| = 2^n - 1$ .*

Although this result is disappointing, Lemmas 6.1 to 6.3 also give us some possible solutions to the problem at hand.

Given a matrix  $\mathbf{A} \in \mathcal{S}^n$  with all off-diagonal entries nonpositive, from Lemma 6.2 we see that we can check if it is copositive by checking if it is positive semidefinite, which can be done very efficiently, for example using the Cholesky algorithm if the matrix is nonsingular. The certificate for being copositive or not, would however be in quite a different form to the certificates considered in the rest of this paper.

An alternative method is given by Algorithm 3, which we can trivially see gives the claimed output by considering Lemmas 6.1 to 6.3.

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**Algorithm 3** Generating certificates to confirm whether or not a matrix with all off-diagonal entries nonpositive is copositive.

---

**Input:**  $\mathbf{X} \in \mathcal{S}^n$  such that  $a_{ij} \leq 0$  for all  $i \neq j$ .

**Output:** Either:

- i.  $\mathbf{v} \in \mathbb{R}_+^n$  such that  $\mathbf{v}^\top \mathbf{X}\mathbf{v} < 0$  (certifying that  $\mathbf{A} \notin \mathcal{COP}^n$ ), or
  - ii.  $\mathbf{u} \in \mathbb{R}_{++}^n$  such that  $\mathbf{X}\mathbf{u} \in \mathbb{R}_+^n$  (certifying that  $\mathbf{X} \in \mathcal{COP}^n$ ).
- 1: Let  $\mathbf{u} = \mathbf{0}_n$  and let  $\mathcal{I}_1, \dots, \mathcal{I}_m \subseteq [1:n]$  be the connected components of  $G_{\mathbf{X}}$ .
  - 2: **for**  $i \in [1:m]$  **do**
  - 3:   Input  $\mathbf{X}_{\mathcal{I}}$  into Algorithm 2 and let  $\mathbf{w} \in \mathbb{R}^{|\mathcal{I}|}$  be the output.
  - 4:   **if**  $\mathbf{w} \in \mathbb{R}_{++}^{|\mathcal{I}_i|}$  **then**
  - 5:      $\mathbf{u} \leftarrow \mathbf{u} + \mathbf{w}_{-\mathcal{I}_i}$
  - 6:   **else if**  $\mathbf{A}_{\mathcal{I}_i} \mathbf{w} \in \mathbb{R}_{++}^{|\mathcal{I}_i|}$  **then**
  - 7:     Let  $\mathbf{v} \in \mathbb{R}_+^n$  such that  $v_i = \max\{0, -(\mathbf{w}_{-\mathcal{I}_i})_i\}$  for all  $i$  and **exit**.
  - 8:   **else**
  - 9:     Let  $\mathbf{y} \in \mathbb{R}_{++}^{|\mathcal{I}_i|}$  be an eigenvector of  $\mathbf{X}_{|\mathcal{I}_i|}$ , let  $\mathbf{v} = \mathbf{y}_{-\mathcal{I}_i}$  and **exit**.
  - 10:   **end if**
  - 11: **end for**
- 

This second method can be extended to more general matrices using the following result, which has a constructive proof for generating such certificates.

**Theorem 6.5.** *For  $\mathbf{X} \in \mathcal{S}^n$  we have that  $\mathbf{X} \in \mathcal{COP}^n$  if and only if there exist sets  $\mathcal{U} \subseteq \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  and  $\mathcal{W} \subseteq \mathbb{R}_+^n$  such that*

- i.  $\forall \mathbf{u} \in \mathcal{U} \cup \mathcal{W}$  we have  $\text{supp}(\mathbf{u}) \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ .
- ii.  $\forall \mathbf{u} \in \mathcal{W}$  and all  $i, j \in \text{supp}(\mathbf{u})$  with  $i \neq j$  we have  $x_{ij} \leq 0$ .
- iii.  $\forall \mathcal{I} \in \mathbb{P}[n]$  s.t.  $\mathbf{X}_{\mathcal{I}}$  is a Z-matrix,  $\exists \mathbf{u} \in \mathcal{W}$  with  $\mathcal{I} \subseteq \text{supp}(\mathbf{u})$ .
- iv.  $\forall \mathcal{I} \in \mathbb{P}[n]$  s.t.  $\mathbf{X}_{\mathcal{I}}$  is not a Z-matrix,  $\exists \mathbf{u} \in (\mathcal{W} \cup \mathcal{U})$  with  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ .

*Proof.* Consider an arbitrary  $\mathcal{I} \in \mathbb{P}[n]$ .

First suppose that  $\mathbf{X}_{\mathcal{I}}$  is not a Z-matrix. If  $\mathbf{X} \in \mathcal{COP}^n$  then by Lemma 4.4,  $\exists \mathbf{y} \in \mathbb{R}^{\mathcal{I}} \setminus (-\mathbb{R}_+^{|\mathcal{I}|})$  such that  $\mathbf{X}_{\mathcal{I}}\mathbf{y} \in \mathbb{R}_+^{|\mathcal{I}|}$  (which we can find using Algorithm 2), and letting  $\mathbf{u} = \mathbf{y}_{-\mathcal{I}} \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  we have  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ . If on the other hand  $\exists \mathbf{u} \in \mathbb{R}^n \setminus (-\mathbb{R}_+^n)$  such that  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$  then by considering  $\mathbf{u}_{\mathcal{I}}$ , from Lemma 4.4 we see that either  $\mathbf{X}_{\mathcal{I}} \in \mathcal{COP}^{|\mathcal{I}|}$  or  $|\mathcal{I}| \geq 2$  and  $\exists i \in \mathcal{I}$  such that  $\mathbf{X}_{\mathcal{I} \setminus \{i\}} \notin \mathcal{COP}^{|\mathcal{I}|}$ .

Now suppose that  $\mathbf{X}_{\mathcal{I}}$  is a Z-matrix. If  $\mathbf{X} \in \mathcal{COP}^n$ , then letting  $\mathcal{J}$  be a maximal set such that  $\mathcal{I} \subseteq \mathcal{J} \subseteq [1:n]$  and  $\mathbf{X}_{\mathcal{J}}$  is a Z-matrix, by Lemma 6.2,  $\exists \mathbf{y} \in \mathbb{R}_{++}^{|\mathcal{J}|}$  such that  $\mathbf{X}_{\mathcal{J}}\mathbf{y} \in \mathbb{R}_{++}^{|\mathcal{J}|}$  (which we can find using Algorithm 3) and letting  $\mathbf{u} = \mathbf{y}_{-\mathcal{J}} \in \mathbb{R}_+^n$ , we have  $\mathcal{I} \subseteq \text{supp}(\mathbf{u}) \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ . If on the other hand  $\exists \mathbf{u} \in \mathbb{R}_+^n$  such that  $\mathcal{I} \subseteq \text{supp}(\mathbf{u}) =: \mathcal{J}$ ,  $\mathbf{X}_{\mathcal{J}}$  is a Z-matrix and  $\mathbf{X}_{\mathcal{J}}\mathbf{u}_{\mathcal{J}} = (\mathbf{X}\mathbf{u})_{\mathcal{J}} \in \mathbb{R}_+^{|\mathcal{J}|}$ , then by Lemma 6.2, we have  $\mathbf{X}_{\mathcal{J}} \in \mathcal{COP}^{|\mathcal{J}|}$ , and thus also  $\mathbf{X}_{\mathcal{I}} \in \mathcal{COP}^{|\mathcal{I}|}$ .

We thus see that if  $\mathbf{X} \in \mathcal{COP}^n$  then such sets  $\mathcal{U}, \mathcal{W}$  exist. Conversely, if such sets  $\mathcal{U}, \mathcal{W}$  exist then  $\nexists \mathcal{I} \in \mathbb{P}[n]$  such that  $\mathbf{X}_{\mathcal{I}} \notin \mathcal{COP}^{|\mathcal{I}|}$  and either  $|\mathcal{I}| = 1$  or  $\mathbf{X}_{\mathcal{I} \setminus \{i\}} \in \mathcal{COP}^{|\mathcal{I}|-1}$  for all  $i \in \mathcal{I}$ , and thus  $\mathbf{X} \in \mathcal{COP}^n$ .  $\square$

Note that as before, checking such a certificate only involves matrix multiplication, checking inequality relations and checking inclusion relations.

*example 6.6.* Consider the matrix

$$\mathbf{X} = \begin{pmatrix} 3 & -1 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 & -1 \\ -1 & -1 & 3 & -1 & 3 \\ -1 & -1 & -1 & 3 & 3 \\ -1 & -1 & 3 & 3 & 3 \end{pmatrix}$$

A minimal certificate for  $\mathbf{X}$  being copositive in the form from Theorem 4.6 is as follows, where we have  $|\mathcal{U}| = 19$ :

$$\mathcal{U} = \left\{ \sum_{i \in \mathcal{I}} \mathbf{e}_i : \emptyset \neq \mathcal{I} \subseteq [1:4] \right\} \cup \left\{ \mathbf{e}_5 + \sum_{i \in \mathcal{I}} \mathbf{e}_i : \mathcal{I} \subseteq [1:2] \right\}.$$

A certificate for  $\mathbf{X}$  being copositive in the form from Theorem 6.5 is as follows, where we have  $|\mathcal{U}| = 2$ ,  $|\mathcal{W}| = 2$  and  $|\mathcal{U}| + |\mathcal{W}| = 4$ :

$$\mathcal{U} = \{\mathbf{e}_5 - \mathbf{e}_3, \mathbf{e}_5 - \mathbf{e}_4\}, \quad \mathcal{W} = \{\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 + \mathbf{e}_4, \mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_5\}.$$

This type of certificate could however still result in an exponentially sized certificate, as we will see in the next example.

*example 6.7.* This example is an adaptation of the result for the maximum number of maximal cliques possible in a simple graph from [31].

For  $n \in 3\mathbb{N}$  such that  $n > 3$ , let  $\mathcal{I}_k = \{3k - 2, 3k - 1, 3k\}$  for  $k \in [1:n/3]$ , and let  $\mathbf{X} \in \mathcal{S}^n$  be such that

$$x_{ij} = \begin{cases} n/3 - 1 > 0 & \text{if } i, j \in \mathcal{I}_k \text{ for some } k \in [1:n/3], \\ -1 < 0 & \text{otherwise.} \end{cases}$$

A certificate for  $\mathbf{X}$  being copositive in the form from Theorem 4.6 is given by the set  $\mathcal{U} = \{\sum_{i \in \mathcal{J}} \mathbf{e}_i : |\mathcal{J} \cap \mathcal{I}_k| \leq 1 \text{ for all } k \in [1:n/3]\} \setminus \{\mathbf{0}_n\}$ , for which we have  $|\mathcal{U}| = 4^{n/3} - 1$ .

For a subset  $\mathcal{J} \subseteq [1:n]$  we have that  $\mathbf{X}_{\mathcal{J}}$  is a maximal principal submatrix of  $\mathbf{X}$  with all off diagonal entries negative if and only if  $|\mathcal{J} \cap \mathcal{I}_k| = 1$  for all  $k \in [1:n/3]$ . There are  $3^{n/3}$  such principal submatrices, implying that if  $\mathcal{U}, \mathcal{W}$  certifies  $\mathbf{X}$  to be copositive then  $|\mathcal{U}| + |\mathcal{W}| \geq 3^{n/3}$ .

We saw in Lemma 5.2 that considering the certificate  $\mathcal{U}$  from Theorem 4.6, we have  $\mathcal{V}_{\min}^{\mathbf{X}} \subseteq \mathbb{R}_{++}\mathcal{U}$ . However in the following example we see that for our new certificate from Theorem 6.5, in general we have  $\mathcal{V}_{\min}^{\mathbf{X}} \not\subseteq \mathbb{R}_{++}(\mathcal{U} \cup \mathcal{W})$ .

*example 6.8.* Consider the matrix

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

A certificate for  $\mathbf{X}$  being copositive in the form from Theorem 6.5 is given by  $\mathcal{W} = \{\mathbf{1}_3\}$  and  $\mathcal{U} = \emptyset$ . However we have  $\mathcal{V}_{\min}^{\mathbf{X}} = \mathbb{R}_{++}\{\mathbf{e}_1 + \mathbf{e}_2\}$ .

We can instead recover  $\mathcal{V}_{\min}^{\mathbf{X}}$  through the following result:

**Theorem 6.9.** Consider  $\mathbf{X} \in \mathcal{COP}^n$  and  $\mathcal{U}, \mathcal{W}$  as in Theorem 6.5. Now let

$$\widehat{\mathcal{V}} = \left\{ \begin{array}{l} \mathbf{u} \in \mathcal{U} \cap \mathbb{R}_+^n, \\ \mu \mathbf{u} : \mu \in \mathbb{R}_{++} \text{ and} \\ \mathbf{u}^\top \mathbf{X} \mathbf{u} = 0 \end{array} \right\} \cup \left\{ \begin{array}{l} \mathbf{w} \in \mathcal{W}, \quad \mathcal{I} \text{ is a conected} \\ \mu(\mathbf{w}_{\mathcal{I}})_{-\mathcal{I}} : \text{component of } G_{\mathbf{X}_{\text{supp}(\mathbf{w})}}, \\ (\mathbf{X}\mathbf{w})_{\mathcal{I}} = \mathbf{0}_{|\mathcal{I}|} \text{ and } \mu \in \mathbb{R}_{++} \end{array} \right\}.$$

Then  $\mathcal{V}_{\min}^{\mathbf{X}} \subseteq \widehat{\mathcal{V}} \subseteq \mathcal{V}^{\mathbf{X}}$  and  $\mathcal{V}_{\min}^{\mathbf{X}} = \{\mathbf{u} \in \widehat{\mathcal{V}} : \nexists \mathbf{w} \in \widehat{\mathcal{V}} \text{ with } \text{supp}(\mathbf{w}) \subsetneq \text{supp}(\mathbf{u})\}$ .

*Proof.* It is trivial to see that  $\widehat{\mathcal{V}} \subseteq \mathcal{V}^{\mathbf{X}}$ , and we will now show that  $\mathcal{V}_{\min}^{\mathbf{X}} \subseteq \widehat{\mathcal{V}}$ . From this the characterisation of  $\mathcal{V}_{\min}^{\mathbf{X}}$  directly follows.

Consider an arbitrary  $\mathbf{v} \in \mathcal{V}_{\min}^{\mathbf{X}}$  and let  $\mathcal{I} = \text{supp}(\mathbf{v})$ . We have  $\mathbf{v}_{\mathcal{I}} \in \mathbb{R}_{++}^{|\mathcal{I}|}$  and from [13, Lemmas 2.3 and 2.5] we have  $\mathbf{X}\mathbf{v} \in \mathbb{R}_+^n$  and  $(\mathbf{X}\mathbf{v})_{\mathcal{I}} = \mathbf{0}_{|\mathcal{I}|}$ . If  $\mathbf{X}_{\mathcal{I}}$  is not a Z-matrix, then similarly to in the proof of Lemma 5.2, we can show that there exists a  $\mathbf{u} \in \mathcal{U} \cap \mathbb{R}_+^n$  such that  $\mathbf{u}^\top \mathbf{X} \mathbf{u} = 0$  and  $\mathbf{v} \in \mathbb{R}_{++}\{\mathbf{u}\}$ . From now on suppose that  $\mathbf{X}_{\mathcal{I}}$  is a Z-matrix. We then have that  $\exists \mathbf{w} \in \mathcal{W}$  such that  $\mathcal{I} \subseteq \text{supp}(\mathbf{w}) =: \mathcal{J}$  and  $\mathbf{X}_{\mathcal{J}}\mathbf{w}_{\mathcal{J}} = (\mathbf{X}\mathbf{w})_{\mathcal{J}} \in \mathbb{R}_+^{|\mathcal{J}|}$  and  $\mathbf{X}_{\mathcal{J}}$  is also a Z-matrix.

We will first show that  $\mathcal{I}$  is a connected component of  $G_{\mathbf{X}_{\mathcal{J}}}$ . Suppose for the sake of contradiction that  $\mathcal{I}$  is not a connected component of  $G_{\mathbf{X}_{\mathcal{J}}}$ . This is equivalent to at least one of the following two cases holding, and for both cases we get a contradiction:

1.  $\exists (i, j) \in \mathcal{I} \times (\mathcal{J} \setminus \mathcal{I})$  such that  $x_{ij} < 0$ : Then we get the contradiction

$$0 \leq (\mathbf{X}\mathbf{v})_j = \sum_{k \in \mathcal{I}} \underbrace{x_{jk}}_{\leq 0} \underbrace{v_k}_{> 0} \leq \underbrace{x_{ji}}_{< 0} \underbrace{v_i}_{> 0} < 0.$$

2.  $\exists \widehat{\mathcal{I}} \in \mathbb{P}[n]$  such that  $\widehat{\mathcal{I}} \subsetneq \mathcal{I}$  and  $x_{ij} = 0$  for all  $(i, j) \in \widehat{\mathcal{I}} \times (\mathcal{I} \setminus \widehat{\mathcal{I}})$ : Then letting  $\widehat{\mathbf{v}} = (\mathbf{v}_{\widehat{\mathcal{I}}})_{-\widehat{\mathcal{I}}} \in \mathbb{R}_+^n \setminus \{\mathbf{0}_n\}$  we have that  $\mathbf{v} - \widehat{\mathbf{v}} \in \mathbb{R}_+^n$  and

$$0 \leq \widehat{\mathbf{v}}^\top \mathbf{X} \widehat{\mathbf{v}} = \underbrace{\mathbf{v}^\top \mathbf{X} \mathbf{v}}_{=0} - \underbrace{(\mathbf{v} - \widehat{\mathbf{v}})^\top \mathbf{X} (\mathbf{v} - \widehat{\mathbf{v}})}_{\geq 0} - 2\mathbf{v}^\top \mathbf{X} (\mathbf{v} - \widehat{\mathbf{v}}) \leq -2 \sum_{\substack{i \in \widehat{\mathcal{I}} \\ j \in \mathcal{I} \setminus \widehat{\mathcal{I}}}} \underbrace{x_{ij}}_{=0} v_i v_j = 0.$$

Therefore  $(\mathbf{v} - \widehat{\mathbf{v}}) \in \mathcal{V}^\mathbf{X}$ , contradicting the claim that  $\mathbf{v} \in \mathcal{V}_{\min}^\mathbf{X}$

The following then implies that  $(\mathbf{X}\mathbf{w})_{\mathcal{I}} = \mathbf{0}_{|\mathcal{I}|}$ :

$$0 = \mathbf{w}_{\mathcal{I}}^\top (\mathbf{X}\mathbf{v})_{\mathcal{I}} = \mathbf{w}^\top \mathbf{X} \mathbf{v} - \underbrace{\mathbf{w}_{\mathcal{J} \setminus \mathcal{I}}^\top (\mathbf{X}\mathbf{v})_{\mathcal{J} \setminus \mathcal{I}}}_{=\mathbf{0}_{|\mathcal{J} \setminus \mathcal{I}|}} \geq \underbrace{\mathbf{v}_{\mathcal{I}}^\top}_{\in \mathbb{R}_{++}^{|\mathcal{I}|}} \underbrace{(\mathbf{X}\mathbf{w})_{\mathcal{I}}}_{\in \mathbb{R}_+^{|\mathcal{I}|}} \geq 0.$$

Now letting  $\widehat{\mathbf{w}} = (\mathbf{w}_{\mathcal{I}})_{-\mathcal{I}} \in \mathbb{R}_+^n \setminus \{\mathbf{0}_n\}$ , we have  $\text{supp}(\widehat{\mathbf{w}}) = \mathcal{I}$  and

$$0 = (\mathbf{X}\mathbf{w})_i = \sum_{j \in \mathcal{I}} x_{ij} w_j + \sum_{j \in \mathcal{J} \setminus \mathcal{I}} \underbrace{x_{ij}}_{=0} w_j = (\mathbf{X}_{\mathcal{I}} \mathbf{w}_{\mathcal{I}})_i = (\mathbf{X}_{\mathcal{I}} \widehat{\mathbf{w}}_{\mathcal{I}})_i \quad \text{for all } i \in \mathcal{I}.$$

Therefore  $\mathbf{X}_{\mathcal{I}} \widehat{\mathbf{w}}_{\mathcal{I}} = \mathbf{0}_{|\mathcal{I}|}$ , and by [23, Lemma 3.7] this implies that  $\widehat{\mathbf{w}}_{\mathcal{I}} \in \mathbb{R}_{++}\{\mathbf{v}_{\mathcal{I}}\}$ . Therefore  $\widehat{\mathbf{w}} \in \mathbb{R}_{++}\{\mathbf{v}\}$ , completing the proof.  $\square$

## 7 Some Extremal Copositive matrices of Order 6

We will now demonstrate the combined power of the results of this paper together with those from [15], using the results of these papers to give what as far as we are aware is a newly discovered set of extremal copositive matrices of order 6. In particular we will consider copositive matrices corresponding to case 9 of Hildebrand's list of possible minimal zero patterns for extremal elements of  $\mathcal{COP}^6$  [24]. After permuting the indices and multiplying the matrix before and after by a positive definite diagonal matrix (see e.g. [10, Theorems 4.3(iv) and 4.6(iv)]), this is equivalent to considering matrices  $\mathbf{X} \in \mathcal{COP}^6$  with  $x_{ii} = 1$  for all  $i$  such that

$$\{\text{supp}(\mathbf{v}) : \mathbf{v} \in \mathcal{V}_{\min}^\mathbf{X}\} = \bigcup_{i=1}^2 \left\{ \{i, i+4\} \right\} \cup \bigcup_{i=1}^4 \left\{ \{i, i+1, i+2\} \right\}$$

Using the results of [13] it can be seen that there exists  $\boldsymbol{\theta} \in \mathbb{R}^5$  and  $\boldsymbol{\psi} \in \mathbb{R}^4$  such that

$$\mathbf{X} = \begin{pmatrix} 1 & -\cos \theta_1 & \cos(\theta_1 + \theta_2) & \cos \psi_1 & -1 & \cos \psi_4 \\ -\cos \theta_1 & 1 & -\cos \theta_2 & \cos(\theta_2 + \theta_3) & \cos \psi_2 & -1 \\ \cos(\theta_1 + \theta_2) & -\cos \theta_2 & 1 & -\cos \theta_3 & \cos(\theta_3 + \theta_4) & \cos \psi_3 \\ \cos \psi_1 & \cos(\theta_2 + \theta_3) & -\cos \theta_3 & 1 & -\cos \theta_4 & \cos(\theta_4 + \theta_5) \\ -1 & \cos \psi_2 & \cos(\theta_3 + \theta_4) & -\cos \theta_4 & 1 & -\cos \theta_5 \\ \cos \psi_4 & -1 & \cos \psi_3 & \cos(\theta_4 + \theta_5) & -\cos \theta_5 & 1 \end{pmatrix},$$

$$0 < \theta_i \text{ for all } i \in [1:5], \quad \theta_i + \theta_{i+1} < \pi \text{ for all } i \in [1:4], \quad 0 \leq \psi_i < \pi \text{ for all } i \in [1:4].$$

We will first show that, given these restrictions on  $\boldsymbol{\theta}, \boldsymbol{\psi}$ , we have that  $\mathbf{X} \in \mathcal{COP}^6$  if and only if

$$\left. \begin{aligned} \boldsymbol{\theta} \in \mathbb{R}_{++}^5, \quad \boldsymbol{\psi} \in \mathbb{R}_+^4, \\ \psi_1 \leq \theta_4, \quad \psi_3 \leq \theta_2, \quad \max\{\psi_2, \psi_4\} \leq \min\{\theta_1, \theta_5\}, \\ \theta_1 + \theta_2 + \theta_3 + \theta_4 \leq \pi, \quad \theta_2 + \theta_3 + \theta_4 + \theta_5 \leq \pi. \end{aligned} \right\} \quad (1)$$

We will then show that  $\mathbf{X}$  is an extremal copositive matrix (i.e.  $\mathbf{X} \in \mathcal{COP}^n$  and if  $\mathbf{A}, \mathbf{B} \in \mathcal{COP}^n$  with  $\mathbf{X} = \mathbf{A} + \mathbf{B}$  then  $\mathbf{A}, \mathbf{B} \in \mathbb{R}_+\{\mathbf{X}\}$ ) if and only if

$$\left. \begin{aligned} \boldsymbol{\theta} \in \mathbb{R}_{++}^5, \quad \boldsymbol{\psi} \in \mathbb{R}^4, \quad \theta_1 + \theta_5 \neq \pi, \\ \psi_1 = \theta_4, \quad \psi_3 = \theta_2, \quad \psi_2 = \psi_4 = \min\{\theta_1, \theta_5\}, \\ \theta_1 + \theta_2 + \theta_3 + \theta_4 < \pi, \quad \theta_2 + \theta_3 + \theta_4 + \theta_5 < \pi. \end{aligned} \right\} \quad (2)$$

All the calculations of this paper can be checked using a matlab code available at <http://dickinson.website>.

## 7.1 Necessary for copositivity

First we will show that the conditions (1) are necessary for  $\mathbf{X}$  to be copositive. If  $\mathbf{X} \in \mathcal{COP}^6$  then for  $i \in [1:2]$  it can be seen that  $(\mathbf{e}_i + \mathbf{e}_{i+4}) \in \mathcal{V}^{\mathbf{X}}$  and thus from [1, p.200] we have  $\mathbf{X}(\mathbf{e}_i + \mathbf{e}_{i+1}) \in \mathbb{R}_+^6$  for all  $i \in [1:2]$ . We then have that (1) follows directly from these inequalities and the requirements on  $\boldsymbol{\theta}, \boldsymbol{\psi}$  (using well known results on the sine and cosine functions).

## 7.2 Sufficient for copositivity

We will now use the results of this paper to show that (1) holding implies that  $\mathbf{X} \in \mathcal{COP}^6$ . To do this we let

$$\begin{aligned} \mathbf{v}_i &= \sin \theta_{i+1} \mathbf{e}_i + \sin(\theta_i + \theta_{i+1}) \mathbf{e}_{i+1} + \sin \theta_i \mathbf{e}_{i+2} \in \mathbb{R}_+^6 \quad \text{for } i \in [1:4], \\ \mathcal{U} &= \bigcup_{\substack{i,j \in [1:6]: \\ i < j}} \{\mathbf{e}_i + \mathbf{e}_j\} \cup \bigcup_{i=1}^4 \{\mathbf{v}_i\}. \end{aligned}$$

Note that  $\mathcal{U} \subseteq \mathbb{R}_+^6 \setminus \{\mathbf{0}_6\}$  when (1) holds, and that  $|\mathcal{U}| = 25 < 63 = 2^6 - 1$ .

Using well known results for the sine and cosine functions, for all  $\boldsymbol{\theta}, \boldsymbol{\psi}$  satisfying (1) we have  $\mathbf{X}\mathbf{v}_i \in \mathbb{R}_+^6$  and  $(\mathbf{X}\mathbf{v}_i)_{\{i,i+1,i+2\}} = \mathbf{0}_3$  for all  $i \in [1:4]$ . In Table 2 we will consider some related properties for the  $(\mathbf{e}_i + \mathbf{e}_j)$ 's.

Using these results and Theorem 4.6, it then directly follows that  $\mathbf{X} \in \mathcal{COP}^6$  for all  $\boldsymbol{\theta}, \boldsymbol{\psi}$  satisfying (1). To aid in seeing this, in Table 3, for each index set  $\mathcal{I} \in \mathbb{P}[6]$  we give a  $\mathbf{u} \in \mathcal{U}$  such that  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$ .

## 7.3 Extremal Matrix

Consider  $\boldsymbol{\theta}, \boldsymbol{\psi}$  satisfying (1) and  $\mathbf{X}$  as defined at the start of this section. Without loss of generality (due to symmetry) we will assume that  $\theta_1 \leq \theta_5$ .

First suppose that either  $\psi_1 < \theta_4$  or  $\psi_3 < \theta_2$  or  $\min\{\psi_2, \psi_4\} < \theta_1 = \min\{\theta_1, \theta_5\}$ . Then we can strictly increase at least one of the elements of  $\boldsymbol{\psi}$  such that (1) still holds

$i \in \dots$	$j$	$\subseteq \text{supp}_{\geq 0}(\mathbf{X}(\mathbf{e}_i + \mathbf{e}_j))$	$(\mathbf{e}_i + \mathbf{e}_j)^\top \mathbf{X}(\mathbf{e}_i + \mathbf{e}_j)$
[1:6]	$i$	$\{i\}$	$4 > 0$
[1:5]	$i + 1$	$\{i - 2, i, i + 1, i + 3\} \cap [1:6]$	$2(1 - \cos \theta_i) > 0$
[1:4]	$i + 2$	$\{i - 3, i, i + 2, i + 5\} \cap [1:6]$	$2(1 + \cos(\theta_i + \theta_{i+1})) > 0$
[1:3]	$i + 3$	$\{i, i + 3\}$	$2(1 + \cos \psi_i) > 0$
[1:2]	$i + 4$	[1:6]	0
{1}	6	{1, 6}	$2(1 + \cos \psi_4) > 0$

Table 2: Some properties for the  $(\mathbf{e}_i + \mathbf{e}_j)$ 's which we will use to show copositivity of  $\mathbf{X}$  in Section 7. The set of indices that must be contained in the nonnegative support of  $\mathbf{X}(\mathbf{e}_i + \mathbf{e}_j)$  (i.e. the column “ $\subseteq \text{supp}_{\geq 0}(\mathbf{X}(\mathbf{e}_i + \mathbf{e}_j))$ ”) follow directly from (1), along with well known results for the sine and cosine functions.

$\mathcal{I}$	$\mathbf{u}$
$\mathcal{I} = \{i\}$ for $i \in [1:6]$	$2\mathbf{e}_i$
$\mathcal{I} = \{i, j\}$ for $i, j \in [1:6], i < j$	$\mathbf{e}_i + \mathbf{e}_j$
$\{i, i + 4\} \subseteq \mathcal{I} \subseteq [1:6]$ for $i \in [1:2]$	$\mathbf{e}_i + \mathbf{e}_{i+4}$
$\{i, i + 1, i + 2\} \subseteq \mathcal{I} \subseteq [1:6]$ for $i \in [1:4]$	$\mathbf{v}_i$
$\mathcal{I} = \{i, i + 1, i + 3\}$ for $i \in [1:3]$	$\mathbf{e}_i + \mathbf{e}_{i+1}$
$\mathcal{I} = \{i, i + 2, i + 3\}$ for $i \in [1:3]$	$\mathbf{e}_{i+2} + \mathbf{e}_{i+3}$
$\mathcal{I} = \{1, 3, 6\}$	$\mathbf{e}_1 + \mathbf{e}_3$
$\mathcal{I} = \{1, 4, 6\}$	$\mathbf{e}_4 + \mathbf{e}_6$
$\mathcal{I} = \{1, 3, 4, 6\}$	$\mathbf{e}_3 + \mathbf{e}_4$

Table 3: This table summarises the index sets  $\mathcal{I} \in \mathbb{P}[6]$  and a corresponding  $\mathbf{u} \in \mathcal{U}$  such that we have  $\text{supp}(\mathbf{u}) \subseteq \mathcal{I} \subseteq \text{supp}_{\geq 0}(\mathbf{X}\mathbf{u})$  for the matrix  $\mathbf{X}$  in Section 7, where  $\boldsymbol{\theta}, \boldsymbol{\psi}$  satisfy (1).

to give a new matrix  $\widehat{\mathbf{X}} \in \mathcal{COP}^6$  with  $\mathbf{X} - \widehat{\mathbf{X}} \in \mathcal{N}^6 \setminus (\mathbb{R}\{\mathbf{X}\})$ , and thus  $\mathbf{X}$  can not be extremal in this case.

From now on we assume that (1) holds with all of the  $\psi_i$ 's at their maximum possible values (and  $\theta_1 \leq \theta_5$ ). In other words, we will assume that

$$\left. \begin{aligned} \boldsymbol{\theta} \in \mathbb{R}_{++}^5, \quad \boldsymbol{\psi} \in \mathbb{R}^4, \quad \psi_1 = \theta_4, \quad \psi_3 = \theta_2, \\ \psi_2 = \psi_4 = \theta_1 \leq \theta_5, \quad \theta_2 + \theta_3 + \theta_4 + \theta_5 \leq \pi. \end{aligned} \right\} \quad (3)$$

From the results in [15], in particular Theorem 17, we have the following result.

**Lemma 7.1.** *Consider a matrix  $\mathbf{X} \in \mathcal{COP}^6$  such that  $x_{jk} \neq 0$  for some  $(j, k) \in [1:6]^2$ . Then  $\mathbf{X}$  is extremal if and only if  $\nexists \mathbf{B} \in \mathcal{S}^n \setminus \{\mathbf{O}\}$  with  $b_{jk} = 0$  and  $(\mathbf{B}\mathbf{v})_i = 0$  for all  $\mathbf{v} \in \mathcal{V}_{\min}^{\mathbf{X}}, i \in [1:6]$  with  $(\mathbf{X}\mathbf{v})_i = 0$ .*

Consider an arbitrary  $\mathbf{B} \in \mathcal{S}^6$  such that  $b_{11} = 0$  and  $(\mathbf{B}\mathbf{v})_i = 0$  for all  $\mathbf{v} \in \mathcal{V}_{\min}^{\mathbf{X}}, i \in [1:6]$  with  $(\mathbf{X}\mathbf{v})_i = 0$ . We will show that provided (3) holds, there exists a nonzero solution  $\mathbf{B}$  to this if and only if (2) holds, completing the proof that  $\mathbf{X}$  is extremal if and only if (2) holds.

From the discussions so far in this section, and using Lemma 5.2, along with well known results on the sine and cosine functions, provided that (3) holds, we have

$$\mathcal{V}_{\min}^{\mathbf{X}} = \{\mu(\mathbf{e}_i + \mathbf{e}_{i+4}) : i \in [1:2], \mu > 0\} \cup \{\mu\mathbf{v}_i : i \in [1:4], \mu > 0\},$$



$$\begin{aligned}
(\mathbf{X}\mathbf{v}_i)_j &= 0 && \text{for } i \in [1:4], j \in \{i, i+1, i+2\}, && (\mathbf{X}\mathbf{v}_1)_6 &= 0, \\
(\mathbf{X}(\mathbf{e}_1 + \mathbf{e}_5))_i &= 0 && \text{for } i \in \{1, 2, 4, 5\}, && (\mathbf{X}(\mathbf{e}_2 + \mathbf{e}_6))_i &= 0 && \text{for } i \in \{1, 2, 3, 6\}, \\
(\mathbf{X}\mathbf{v}_2)_6 / \sin \theta_2 &= (\mathbf{X}(\mathbf{e}_2 + \mathbf{e}_6))_4 = \cos(\theta_2 + \theta_3) + \cos(\theta_4 + \theta_5) \geq 0 \\
&&& \text{with equality iff } \theta_2 + \theta_3 + \theta_4 + \theta_5 = \pi, \\
(\mathbf{X}\mathbf{v}_3)_6 &= (\mathbf{X}\mathbf{v}_4)_3 = \sin \theta_4 (\cos \theta_2 + \cos(\theta_3 + \theta_4 + \theta_5)) \geq 0 \\
&&& \text{with equality iff } \theta_2 + \theta_3 + \theta_4 + \theta_5 = \pi, \\
(\mathbf{X}\mathbf{v}_4)_1 / \sin \theta_4 &= (\mathbf{X}(\mathbf{e}_1 + \mathbf{e}_5))_6 = (\mathbf{X}(\mathbf{e}_2 + \mathbf{e}_6))_5 = \cos \theta_1 - \cos \theta_5 \geq 0 \\
&&& \text{with equality iff } \theta_1 = \theta_5, \\
(\mathbf{X}\mathbf{v}_4)_2 &= \sin \theta_5 (\cos(\theta_2 + \theta_3) + \cos(\theta_4 + \theta_5)) + \sin(\theta_4 + \theta_5)(\cos \theta_1 - \cos \theta_5) \geq 0 \\
&&& \text{with equality iff } \theta_1 = \theta_5 = \pi - \theta_2 - \theta_3 - \theta_4, \\
(\mathbf{X}\mathbf{v}_1)_4 &= (\mathbf{X}\mathbf{v}_2)_1 = \sin \theta_2 (\cos(\theta_1 + \theta_2 + \theta_3) + \cos \theta_4) \geq 0 \\
&&& \text{with equality iff } \theta_1 = \theta_5 = \pi - \theta_2 - \theta_3 - \theta_4, \\
(\mathbf{X}\mathbf{v}_1)_5 / \sin \theta_1 &= (\mathbf{X}\mathbf{v}_3)_1 / \sin \theta_4 = (\mathbf{X}(\mathbf{e}_1 + \mathbf{e}_5))_3 = \cos(\theta_1 + \theta_2) + \cos(\theta_3 + \theta_4) \geq 0 \\
&&& \text{with equality iff } \theta_1 = \theta_5 = \pi - \theta_2 - \theta_3 - \theta_4, \\
(\mathbf{X}\mathbf{v}_2)_5 &= (\mathbf{X}\mathbf{v}_3)_2 = \sin \theta_3 (\cos \theta_1 + \cos(\theta_2 + \theta_3 + \theta_4)) \geq 0 \\
&&& \text{with equality iff } \theta_1 = \theta_5 = \pi - \theta_2 - \theta_3 - \theta_4.
\end{aligned}$$

By considering the following requirements on  $B$  we get that each element of  $\mathbf{B}$  can be given as a unique linear function of  $b_{12}$  and  $b_{22}$ :

$$\left. \begin{aligned}
\mathbf{B} &\in \mathcal{S}^6, && b_{11} &= 0, \\
(\mathbf{B}\mathbf{v}_i)_j &= 0 \text{ for all } i \in [1:4], j \in \{i, i+1, i+2\}, \\
(\mathbf{B}(\mathbf{e}_1 + \mathbf{e}_5))_i &= 0 \text{ for all } i \in \{1, 2, 4\}, \\
(\mathbf{B}(\mathbf{e}_2 + \mathbf{e}_6))_i &= 0 \text{ for all } i \in \{1, 2, 3\}.
\end{aligned} \right\} \quad (4)$$

In particular we have

$$\begin{aligned}
b_{15} &= 0, && b_{26} &= -b_{22}, \\
b_{55} &= \frac{\sin \left( \sum_{j=1}^4 \theta_j \right)}{\sin^2 \theta_1} \left( 2b_{12} \sin \left( \sum_{j=2}^4 \theta_j \right) + b_{22} \sin \left( \sum_{j=1}^4 \theta_j \right) \right), \\
b_{66} &= \frac{\sin \left( \sum_{j=1}^5 \theta_j \right)}{\sin^2 \theta_1} \left( 2b_{12} \sin \left( \sum_{j=2}^5 \theta_j \right) + b_{22} \sin \left( \sum_{j=1}^5 \theta_j \right) \right).
\end{aligned}$$

Combining this with the requirements that  $(\mathbf{B}(\mathbf{e}_1 + \mathbf{e}_5))_5 = 0 = (\mathbf{B}(\mathbf{e}_2 + \mathbf{e}_6))_6$  we get

that  $\mathbf{M} \begin{pmatrix} 2b_{12} \\ b_{22} \end{pmatrix} = \mathbf{0}_2$  where

$$\mathbf{M} = \begin{pmatrix} \sin \left( \sum_{j=1}^4 \theta_j \right) \sin \left( \sum_{j=2}^4 \theta_j \right) & \sin^2 \left( \sum_{j=1}^4 \theta_j \right) \\ \sin \left( \sum_{j=1}^5 \theta_j \right) \sin \left( \sum_{j=2}^5 \theta_j \right) & \sin^2 \left( \sum_{j=1}^5 \theta_j \right) - \sin^2 \theta_1 \end{pmatrix},$$

$$\det \mathbf{M} = -\sin(\theta_1) \sin(\theta_1 + \theta_5) \sin \left( \sum_{j=1}^4 \theta_j \right) \sin \left( \sum_{j=2}^5 \theta_j \right).$$

We now finish by considering 3 cases:

1. If (3) holds with  $\theta_1 = \theta_5 = \pi - \theta_2 - \theta_3 - \theta_4$ , then letting  $b_{12} = 0$  and  $b_{22} = 1$ , and letting the other elements of  $\mathbf{B}$  be given by the equations (4) it can be shown that  $\mathbf{B}\mathbf{v} = \mathbf{0}_6$  for all  $\mathbf{v} \in \mathcal{V}_{\min}^{\mathbf{X}}$ , and thus  $\mathbf{X}$  is not extremal in this case.
2. If (3) holds with  $\theta_1 < \pi - \theta_2 - \theta_3 - \theta_4$  and  $(\pi - \theta_5) \in \{\theta_1, \theta_2 + \theta_3 + \theta_4\}$ , then letting  $b_{12} = \sin \left( \sum_{j=1}^4 \theta_j \right) \neq 0$  and  $b_{22} = -2 \sin \left( \sum_{j=2}^4 \theta_j \right) \neq 0$ , and letting the other elements of  $\mathbf{B}$  be given by the equations (4) it can be shown that  $(\mathbf{B}\mathbf{v})_i = 0$  for all  $\mathbf{v} \in \mathcal{V}_{\min}^{\mathbf{X}}$  and  $i \in [1:6]$  with  $(\mathbf{X}\mathbf{v}_i) = 0$ , and thus  $\mathbf{X}$  is also not extremal in this case.
3. If (3) holds with  $\theta_1 + \theta_5 \neq \pi$  and  $\theta_1 \leq \theta_5 < \pi - \theta_2 - \theta_3 - \theta_4$  then we have  $\det \mathbf{M} \neq 0$ , and thus  $b_{12} = b_{22} = 0$ . Therefore  $\mathbf{B} = \mathbf{O}$  in this case. This completes the proof that  $\mathbf{X}$  is extremal if and only if (2) holds.

## 8 Conclusion

In this article, we introduced a new way of certifying a matrix to be copositive. This certificate is constructed through solving finitely many linear systems, and is checked by checking finitely many linear inequalities. In some cases this certificate can be relatively small, even when the matrix generates an extreme ray of the copositive cone which is not positive semidefinite plus nonnegative. Unfortunately, in general the certificate can be exponentially large, however this is only to be expected as the problem of checking copositivity is a co-NP-complete problem. This certificate is useful not only in proving the matrix to be copositive, but also in generating its set of minimal zeros which can then be used to analyse properties of this copositive matrix.

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## References

- [1] Leonard D. Baumert. Extreme copositive quadratic forms. *Pacific Journal of Mathematics*, 19:197–204, 1966.

- [2] Abraham Berman and Robert J. Plemmons. *Nonnegative Matrices in the Mathematical Sciences*. SIAM, 1994.
- [3] Immanuel M. Bomze and Etienne de Klerk. Solving standard quadratic optimization problems via linear, semidefinite and copositive programming. *Journal of Global Optimization*, 24(2):163–185, 2002.
- [4] Immanuel M. Bomze and Gabriele Eichfelder. Copositivity detection by difference-of-convex decomposition and  $\omega$ -subdivision. *Mathematical Programming*, 138(12):365–400, 2013.
- [5] Immanuel M. Bomze, Werner Schachinger, and Gabriele Uchida. Think co(mpletely )positive! matrix properties, examples and a clustered bibliography on copositive optimization. *Journal of Global Optimization*, 52(3):423–445, 2012.
- [6] Stefan Bundfuss and Mirjam Dür. Algorithmic copositivity detection by simplicial partition. *Linear Algebra and its Applications*, 428:1511–1523, 2008.
- [7] Samuel Burer. *Copositive Programming*, Miguel F. Anjos and Jean B. Lasserre (Eds.), volume 166 of *International Series in Operations Research & Management Science*, pages 201–218. Springer US, 2012.
- [8] Palahenedi H. Diananda. On a conjecture of l. j. mordell regarding an inequality involving quadratic forms. *Journal of the London Mathematical Society*, s1-36(1):185–192, 1961.
- [9] Palahenedi H. Diananda. On nonnegative forms in real variables some or all of which are nonnegative. *Mathematical Proceedings of the Cambridge Philosophical Society*, 58:17–25, 1962.
- [10] Peter J.C. Dickinson. Geometry of the copositive and completely positive cones. *Journal of Mathematical Analysis and Applications*, 380(1):377–395, 2011.
- [11] Peter J.C. Dickinson. *The Copositive Cone, the Completely Positive Cone and their Generalisations*. PhD thesis, University of Groningen, 2013.
- [12] Peter J.C. Dickinson. On the exhaustivity of simplicial partitioning. *Journal of Global Optimization*, 58(1):189–203, 2014.
- [13] 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.
- [14] Peter J.C. Dickinson, Mirjam Dür, Luuk Gijben, and Roland Hildebrand. Scaling relationship between the copositive cone and Parrilo’s first level approximation. *Optimization Letters*, 7(8):1669–1679, 2013.
- [15] Peter J.C. Dickinson and Roland Hildebrand. Considering copositivity locally. *Journal of Mathematical Analysis and Applications*, 437(2):1184–1195, 2016.
- [16] Peter J.C. Dickinson and Janez Povh. Moment approximations for set-semidefinite polynomials. *Journal of Optimization Theory and Applications*, 159(1):57–68, 2013.

- [17] Peter J.C. Dickinson and Janez Povh. On an extension of pólya’s positivstellensatz. *Journal of Global Optimization*, 61(4):615–625, 2015.
- [18] Mirjam Dür. *Copositive Programming - a Survey*, Moritz Diehl, Francois Glineur, Elias Jarlebring and Wim Michiels (Eds.), pages 3–20. Springer Berlin Heidelberg, 2010.
- [19] Julius Farkas. Über die theorie der einfachen ungleichungen. *Journal für die Reine und Angewandte Mathematik*, 124:1–24, 1902.
- [20] Karl-Peter Hadeler. On copositive matrices. *Linear Algebra and its Applications*, 49:79–89, 1983.
- [21] Godfrey Harold Hardy, John Edensor Littlewood, and George Pólya. *Inequalities*. Cambridge University Press, 1988.
- [22] Emilie Haynsworth and Alan J. Hoffman. Two remarks on copositive matrices. *Linear Algebra and its Applications*, 2:387–392, 1969.
- [23] Roland Hildebrand. Minimal zeros of copositive matrices. *Linear Algebra and its Applications*, 459:154–174, 2014.
- [24] Roland Hildebrand. Copositive matrices of size  $6 \times 6$ . <http://www-ljk.imag.fr/membres/Roland.Hildebrand/c6classification/c6.htm>, as of 2nd March 2018.
- [25] Alan J. Hoffman and Francisco Pereira. On copositive matrices with -1,0,1 entries. *Journal of Combinatorial Theory*, 14(3):302–309, 1973.
- [26] John E. Hopcroft, Rajeev Motwani, and Jeffrey D. Ullman. *Introduction to Automata Theory, Languages, and Computation, 2nd Ed.* Pearson, 2nd edition edition, 2000.
- [27] Wilfred Kaplan. A test for copositive matrices. *Linear Algebra and its Applications*, 313(1-3):203–206, 2000.
- [28] Jean B. Lasserre. A new look at nonnegativity on closed sets and polynomial optimization. *SIAM Journal on Optimization*, 21(3):864–885, 2011.
- [29] W. Mantel. Problem 28. *Wiskundige Opgaven*, 10:60–61, 1907.
- [30] John E. Maxfield and Henryk Minc. On the matrix equation  $X'X = A$ . *Proceedings of the Edinburgh Mathematical Society (Series 2)*, 13(02):125–129, 1962.
- [31] John W. Moon and Leo Moser. On cliques in graphs. *Israel journal of Mathematics*, 3(1):2328, 1965.
- [32] Katta G. Murty and Santosh N. Kabadi. Some np-complete problems in quadratic and nonlinear programming. *Mathematical Programming*, 39(2):117–129, 1987.
- [33] Pablo A Parrilo. *Structured semidefinite programs and semialgebraic geometry methods in robustness and optimization*. PhD thesis, California Institute of Technology, 2000.

- [34] Javier F. Peña, Juan C. Vera, and Luis F. Zuluaga. Computing the stability number of a graph via linear and semidefinite programming. *SIAM Journal on Optimization*, 18(1):87–105, 2007.
- [35] Li Ping and Feng Yu Yu. Criteria for copositive matrices of order four. *Linear Algebra and its Applications*, 194:109–124, 1993.
- [36] Arie J. Quist, Etienne de Klerk, Cornelis Roos, and Tamàs Terlaky. Copositive relaxation for general quadratic programming. *Optimization Methods and Software*, 9:185–208, 1998.
- [37] Naomi Shaked-Monderer, Abraham Berman, Mirjam Dür, and M. Rajesh Kannan. SPN completable graphs. *Linear Algebra and its Applications*, 498:58–73, 2016.

## A Proofs for Section 6

*Proof of Lemma 6.1.* Let  $\mu = \max\{a_{ii} : i \in [1:n]\}$  and let  $\mathbf{B} = \mu\mathbf{I}_n - \mathbf{A}$ . We have that  $\mathbf{B} \in \mathcal{N}^n$  and  $G_{\mathbf{B}} = G_{\mathbf{A}}$  is connected. Therefore, by the Perron-Frobenius theorem [2, Theorems 2.1.1 and 2.1.4], there exists an eigenvector  $\mathbf{w} \in \mathbb{R}_{++}^n$  of  $\mathbf{B}$  with corresponding eigenvalue  $\nu > 0$  of geometric multiplicity one such that all the other eigenvalues of  $\mathbf{B}$  are between  $-\nu$  and  $\nu$ . Therefore  $\mathbf{w}$  is an eigenvector of  $\mathbf{A}$  with corresponding eigenvalue  $\lambda := \mu - \nu$  of geometric multiplicity one, with all other eigenvalues of  $\mathbf{A}$  being between  $\lambda$  and  $\lambda + 2\nu$ .

If  $\lambda \geq 0$  then we have  $\mathbf{A} \in \mathcal{PSD}^n \subseteq \mathcal{COP}^n$ . Conversely, if  $\lambda < 0$  then  $\mathbf{w} \in \mathbb{R}_{++}^n$  and  $\mathbf{w}^T \mathbf{A} \mathbf{w} = \lambda \|\mathbf{w}\|_2^2 < 0$ , implying that  $\mathbf{A} \notin \mathcal{COP}^n$ .  $\square$

*Proof of Lemma 6.2.* It was shown in [35, Theorem 4] that 2 implies 1.

Now suppose that 3 holds. Then for all  $\varepsilon > 0$  we have that  $(\mathbf{A} + \varepsilon\mathbf{I})$  has all off-diagonal entries nonpositive and  $(\mathbf{A} + \varepsilon\mathbf{I})\mathbf{x} \in \mathbb{R}_{++}^n$ . By the results of [2, Chapter 6], in particular case (I<sub>27</sub>), we thus have that  $\mathbf{A} + \varepsilon\mathbf{I}$  is a positive definite matrix. As the set of positive semidefinite matrices is closed, this implies that 2 holds.

Finally suppose that 1 holds. Let  $\mathcal{I}_1, \dots, \mathcal{I}_m$  be the connected components of  $G_{\mathbf{A}}$ . For all  $i \in [1:m]$  we have  $\mathbf{A}_{\mathcal{I}_i} \in \mathcal{COP}^{|\mathcal{I}_i|}$ , and thus by Lemma 6.1 there exists an eigenvector of  $\mathbf{A}_{\mathcal{I}_i}$  given by  $\mathbf{y}^i \in \mathbb{R}_{++}^{|\mathcal{I}_i|}$  with corresponding eigenvalue  $\lambda_i \geq 0$ . From the definition of  $\mathcal{I}_i$ , we thus have  $\text{supp}(\mathbf{A}\mathbf{y}_{-\mathcal{I}_i}^i) \subseteq \mathcal{I}_i$  and thus  $\mathbf{A}\mathbf{y}_{-\mathcal{I}_i}^i \in \mathbb{R}_+^n$ . Letting  $\mathbf{x} = \sum_{i=1}^m \mathbf{y}_{-S\mathcal{I}_i}^i \in \mathbb{R}_{++}^n$ , we then have  $\mathbf{A}\mathbf{x} = \sum_{i=1}^m \mathbf{A}\mathbf{y}_{-S\mathcal{I}_i}^i \in \mathbb{R}_+^n$ .  $\square$