

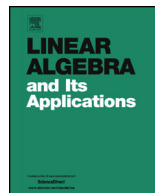


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On the exactness of sum-of-squares approximations for the cone of 5×5 copositive matrices [☆]Monique Laurent ^{a,b}, Luis Felipe Vargas ^{a,*}^a *Centrum Wiskunde & Informatica (CWI), Amsterdam, Netherlands*^b *Tilburg University, Netherlands*

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ABSTRACT

We investigate the hierarchy of conic inner approximations $\mathcal{K}_n^{(r)}$ ($r \in \mathbb{N}$) for the copositive cone COP_n , introduced by Parrilo (2000) [22]. It is known that $\text{COP}_4 = \mathcal{K}_4^{(0)}$ and that, while the union of the cones $\mathcal{K}_n^{(r)}$ covers the interior of COP_n , it does not cover the full cone COP_n if $n \geq 6$. Here we investigate the remaining case $n = 5$, where all extreme rays have been fully characterized by Hildebrand (2012) [12]. We show that the Horn matrix H and its positive diagonal scalings play an exceptional role among the extreme rays of COP_5 . We show that equality $\text{COP}_5 = \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ holds if and only if every positive diagonal scaling of H belongs to $\mathcal{K}_5^{(r)}$ for some $r \in \mathbb{N}$. As a main ingredient for the proof, we introduce new Lasserre-type conic inner approximations for COP_n , based on sums of squares of polynomials. We show their links to the cones $\mathcal{K}_n^{(r)}$, and we use an optimization approach that permits to exploit finite convergence results on Lasserre hierarchy to show membership in the new cones.

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* Corresponding author.

E-mail addresses: monique.laurent@cwi.nl (M. Laurent), luis.vargas@cwi.nl (L.F. Vargas).

1. Introduction

The main object of study in this paper is the cone of copositive matrices COP_n , defined as

$$\text{COP}_n = \{M \in \mathcal{S}^n : x^T M x \geq 0 \text{ for all } x \in \mathbb{R}_+^n\} \quad (1.1)$$

or, equivalently, as

$$\text{COP}_n = \{M \in \mathcal{S}^n : (x^{\circ 2})^T M x^{\circ 2} \geq 0 \text{ for all } x \in \mathbb{R}^n\}, \quad (1.2)$$

after setting $x^{\circ 2} = (x_1^2, \dots, x_n^2)$ and $\mathbb{R}_+^n = \{x \in \mathbb{R}^n : x \geq 0\}$. Optimizing over the copositive cone is hard in general since this captures a wealth of hard combinatorial optimization problems such as finding maximum stable sets in graphs and minimum graph coloring, and, more generally, mixed-integer binary optimization problems (see, e.g., [2], [10], [3], [8]). Determining whether a matrix M is copositive is a co-NP-complete problem (see [20]). These hardness results motivate investigating hierarchies of cones that offer tractable approximations for the copositive cone. Such conic approximations arise naturally by replacing the condition $x^T M x \geq 0$ on \mathbb{R}_+^n in (1.1), or the condition $(x^{\circ 2})^T M x^{\circ 2} \geq 0$ on \mathbb{R}^n in (1.2), by a *sufficient* condition for nonnegativity. Parrilo [22] introduced the cones $\mathcal{K}_n^{(r)}$, whose definition relies on requiring that the polynomial $(\sum_{i=1}^n x_i^2)^r (x^{\circ 2})^T M x^{\circ 2}$ is a sum of squares of polynomials, i.e.,

$$\mathcal{K}_n^{(r)} = \left\{ M \in \mathcal{S}^n : \left(\sum_{i=1}^n x_i^2 \right)^r (x^{\circ 2})^T M x^{\circ 2} \in \Sigma \right\}. \quad (1.3)$$

Here and throughout, $\Sigma = \{\sum_i q_i^2 : q_i \in \mathbb{R}[x]\}$ denotes the cone of sums of squares of polynomials, $\mathbb{R}[x]_r$ denotes the space of polynomials with degree at most r , and we set $\Sigma_r = \Sigma \cap \mathbb{R}[x]_r$. By construction we have $\mathcal{K}_n^{(r)} \subseteq \mathcal{K}_n^{(r+1)} \subseteq \text{COP}_n$ and thus

$$\bigcup_{r \geq 0} \mathcal{K}_n^{(r)} \subseteq \text{COP}_n. \quad (1.4)$$

In addition, the cones $\mathcal{K}_n^{(r)}$ cover the interior of the copositive cone, i.e.,

$$\text{int}(\text{COP}_n) \subseteq \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}. \quad (1.5)$$

Indeed, a matrix M lies in the interior of COP_n precisely when $x^T M x > 0$ on $\mathbb{R}_+^n \setminus \{0\}$, or, equivalently, when $(x^{\circ 2})^T M x^{\circ 2} > 0$ on $\mathbb{R}^n \setminus \{0\}$. Using a result of Pólya [24] (or Reznick [26]), this strict positivity condition implies existence of an integer $r \in \mathbb{N}$ for which $(\sum_{i=1}^n x_i^2)^r (x^{\circ 2})^T M x^{\circ 2}$ is a sum of squares.

As is well-known, the cone $\mathcal{K}_n^{(0)}$ consists of the matrices that can be written as the sum of a positive semidefinite matrix and a nonnegative matrix, thus it is the dual cone of the doubly-nonnegative cone (see [22]). We have equality $\text{COP}_n = \mathcal{K}_n^{(0)}$ if and only if $n \leq 4$ [4]. For $n \geq 6$, copositive matrices that do not belong to any cone $\mathcal{K}_n^{(r)}$ have been constructed in [17], so the inclusion (1.4) is strict for any $n \geq 6$. However, the question of deciding whether the inclusion (1.4) is strict for $n = 5$, which is the main topic of this paper, remains open.

Question 1.1 ([17]). Does equality $\text{COP}_5 = \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ hold?

It is known that the inclusion $\mathcal{K}_5^{(0)} \subseteq \text{COP}_5$ is strict. For instance, the following matrix, known as the *Horn matrix*,

$$H = \begin{pmatrix} 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 \end{pmatrix} \quad (1.6)$$

is copositive, but it does not belong to the cone $\mathcal{K}_5^{(0)}$. On the other hand, H belongs to the cone $\mathcal{K}_5^{(1)}$ (see [22]). Clearly, any positive diagonal scaling of a copositive matrix remains a copositive matrix, i.e., $M \in \text{COP}_n$ implies $DMD \in \text{COP}_n$ for any diagonal matrix D with $D_{ii} > 0$ for $i \in [n]$. However, this operation does *not* preserve the cone $\mathcal{K}_n^{(r)}$ for $r \geq 1$ (see [5]). For instance, $H \in \mathcal{K}_5^{(1)}$, but not every positive diagonal scaling of H belongs to $\mathcal{K}_5^{(1)}$; in fact the positive diagonal scalings of H that still belong to $\mathcal{K}_5^{(1)}$ are characterized in [17]. It is an open question whether every positive diagonal scaling of H belongs to some cone $\mathcal{K}_5^{(r)}$.

Question 1.2. Is it true that $DHD \in \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ for all positive diagonal matrices D ?

As we will show in this paper, a positive answer to Question 1.2 would imply a positive answer to Question 1.1. The following is the main contribution of this paper.

Theorem 1.3. Equality $\text{COP}_5 = \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ holds if and only if $DHD \in \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ for all positive diagonal matrices D .

We group a few observations regarding the proof of this result. In view of relation (1.5), in order to show that any 5×5 copositive matrix lies in some cone $\mathcal{K}_5^{(r)}$, we can restrict our attention to copositive matrices that lie on the boundary ∂COP_5 of the copositive cone. Moreover, it suffices to consider matrices that lie on an extreme ray of COP_5 . A crucial ingredient for the proof of Theorem 1.3 is the fact that all the extreme rays of the cone COP_5 are known. They have been characterized by Hildebrand [12], who proved that (up to simultaneous row/column permutation) they fall into three categories: either

they are generated by a matrix in $\mathcal{K}_5^{(0)}$, or they are generated by a positive diagonal scaling of the Horn matrix, or they are generated by a positive diagonal scaling of a class of special matrices $T(\psi)$ (see Theorem 2.2 below for details). Hence, in order to show Theorem 1.3, we need to show that all positive diagonal scalings of the matrices $T(\psi)$ lie in some cone $\mathcal{K}_5^{(r)}$. This forms the main technical part of the paper, which, as we will explain later in Section 4, relies on following an optimization approach.

We now place the above results into the broader context of the relevant literature.

On the impact of diagonal scaling

Diagonal scaling plays a crucial role in our main result (Theorem 1.3) and more generally in the analysis of the copositive cone. As already noted above, positive diagonal scaling preserves the copositive cone COP_n . It also preserves the cone $\mathcal{K}_n^{(0)}$, but it does not preserve the cone $\mathcal{K}_n^{(r)}$ when $r \geq 1$ and $n \geq 5$. Indeed, Dickinson et al. [5] show that, for every matrix $M \in \text{COP}_n \setminus \mathcal{K}_n^{(0)}$ and every $r \in \mathbb{N}$, there exists a positive diagonal scaling of M that does not belong to $\mathcal{K}_n^{(r)}$.

On the other hand, it is shown in [5] that every 5×5 copositive matrix with an all-ones diagonal belongs to $\mathcal{K}_5^{(1)}$. Hence, a method for checking whether a 5×5 matrix belongs to COP_5 is to scale it to obtain a matrix with binary diagonal entries and then to check whether this new matrix belongs to $\mathcal{K}_5^{(1)}$. In contrast, it is shown in [17] that, for every $n \geq 7$, there exist matrices in $\text{COP}_n \setminus \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$ with an all-ones diagonal; indeed, if $M \in \text{COP}_n \setminus \mathcal{K}_n^{(0)}$, then

$$M \oplus \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \in \text{COP}_{n+2} \setminus \bigcup_{r \geq 0} \mathcal{K}_{n+2}^{(r)}.$$

Selecting for M the Horn matrix H gives a 7×7 copositive matrix that does not belong to any cone $\mathcal{K}_7^{(r)}$. The case $n = 6$ remains open.

Question 1.4. Let $M \in \text{COP}_6$ with an all-ones diagonal. Does it hold that $M \in \bigcup_{r \geq 0} \mathcal{K}_6^{(r)}$?

Note that the answer to this question is negative in general if we allow M to have a zero diagonal entry. Indeed, it is shown in [17] that, if $M \in \text{COP}_n \setminus \mathcal{K}_n^{(0)}$, then the matrix $M \oplus 0$ is copositive but does not belong to any cone $\mathcal{K}_{n+1}^{(r)}$. So selecting $M = H$ gives the 6×6 matrix $H \oplus 0$, which is copositive but does not belong to any cone $\mathcal{K}_6^{(r)}$.

Copositive matrices from graphs

The cones $\mathcal{K}_n^{(r)}$ are used by de Klerk and Pasechnik [10] for defining a hierarchy of upper bounds $\vartheta^{(r)}(G)$ for the stability number $\alpha(G)$ of a graph $G = (V = [n], E)$. Recall $\alpha(G)$ denotes the maximum cardinality of a set $S \subseteq V$, which is stable (aka independent), i.e., contains no edge of G . The parameter $\vartheta^{(r)}(G)$ is defined as the smallest scalar λ

such that $\lambda(I + A_G) - J \in \mathcal{K}_n^{(r)}$. Here, A_G is the adjacency matrix of G , I is the identity matrix and J is the all-ones matrix. As an application of a result of Motzkin-Straus [19], it follows that the following *graph matrix* $M_G := \alpha(G)(I + A_G) - J$ is copositive. Hence, the parameters $\vartheta^{(r)}(G)$ provide a hierarchy of upper bounds for $\alpha(G)$, converging to it asymptotically [10]. The authors conjecture in [10] that the convergence is, in fact, finite and takes place after $\alpha(G)$ steps, i.e., they conjecture that $\vartheta^{(r)}(G) = \alpha(G)$ if $r \geq \alpha(G) - 1$ or, equivalently, that the matrix M_G belongs to the cone $\mathcal{K}_n^{(\alpha(G)-1)}$. In fact, it is not even known whether M_G belongs to *some* cone $\mathcal{K}_n^{(r)}$. So the following two conjectures remain open.

Conjecture 1.5 ([10]). *For any graph G , we have $M_G \in \mathcal{K}_n^{(\alpha(G)-1)}$.*

Conjecture 1.6 ([16]). *For any graph G , we have $M_G \in \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$.*

The class of graph matrices M_G has been recently further investigated in [7], where they are used, in particular, to construct large classes of matrices generating extreme rays of COP_n .

A possible strategy for attacking the above conjectures is to use hierarchies of subcones of the cones $\mathcal{K}_n^{(r)}$, that have additional structural properties and thus may be easier to handle. The starting point to define such subcones is to use the formulation (3.2), which characterizes membership $M \in \mathcal{K}_n^{(r)}$ by a structured decomposition for the polynomial $(\sum_i x_i)^r x^T M x$. Then, by restricting the summation in (3.2) to selected summands, one gets subcones of $\mathcal{K}_n^{(r)}$.

Peña et al. [23] introduce the cones $\mathcal{Q}_n^{(r)} \subseteq \mathcal{K}_n^{(r)}$, as defined in (3.7), and show that $M_G \in \mathcal{Q}_n^{(\alpha(G)-1)}$ for all graphs G with $\alpha(G) \leq 6$. Laurent and Gvozdenović [11] strengthen this and show $M_G \in \mathcal{Q}_n^{(\alpha(G)-1)}$ for all graphs with $\alpha(G) \leq 8$, which settles Conjecture 1.5 for the class of graphs with $\alpha(G) \leq 8$. Very roughly, the cones $\mathcal{Q}_n^{(r)}$ allow an inductive proof, by combining with combinatorial properties of the graph matrices M_G ; however this argument breaks down when $\alpha(G) \geq 9$. So a new strategy seems needed to attack Conjecture 1.5 for general graphs.

In this paper, we introduce another class of cones $\text{LAS}_{\Delta_n}^{(r)} \subseteq \mathcal{K}_n^{(r)}$ (see (2.3)), which we use to establish our main result (Theorem 1.3). Roughly, these cones are based on following an optimization approach, where one minimizes the quadratic form $x^T M x$ over the standard simplex, and then considers the associated Lasserre-type sum-of-squares hierarchy, which allows applying known results about their finite convergence.

We have (implicitly) used the cones $\text{LAS}_{\Delta_n}^{(r)}$ already in our previous work [16] to prove a partial result on Conjecture 1.6. Call an edge e of G *critical* if its deletion increases the stability number, i.e., if $\alpha(G \setminus e) = \alpha(G) + 1$. Now we say that G is *critical* if all its edges are critical, and that G is *acritical* if none of its edges is critical. In [16] it is shown that, if G is acritical, then M_G belongs to some cone $\text{LAS}_n^{(r)} \subseteq \mathcal{K}_n^{(r)}$.

Observe that the Horn matrix coincides with the graph matrix M_{C_5} of the 5-cycle. As C_5 is a critical graph, the above mentioned result of [16] does not apply to it. In

fact, we will show in Lemma 3.10 that $H = M_{C_5} \notin \bigcup_{r \geq 0} \text{LAS}_5^{(r)}$. So we cannot use the cones $\text{LAS}_n^{(r)}$ to show membership in the cones $\mathcal{K}_n^{(r)}$ of the positive diagonal scalings of H . Recall that $H \in \mathcal{K}_5^{(1)}$. However, as positive diagonal scaling does not preserve the cone $\mathcal{K}_n^{(r)}$ in general, we will need another strategy to show that every positive diagonal scaling of H belongs to some $\mathcal{K}_5^{(r)}$.

Organization of the paper

The paper is organized as follows. In Section 2 we give an overview of the main tools and results: we introduce other sum-of-squares hierarchies of inner approximations for COP_n (including the cones $Q_n^{(r)}$ and $\text{LAS}_n^{(r)}$), we present the known description of the extreme rays of COP_5 (that include the matrices $T(\psi)$ ($\psi \in \Psi$) from (2.7)), and we sketch the main arguments used to show the main result (Theorem 1.3). As we explain there, Theorem 1.3 reduces to showing that every positive diagonal scaling of the matrices $T(\psi)$ ($\psi \in \Psi$) belongs to some of the cones $\text{LAS}_n^{(r)}$ (Theorem 2.3). In Section 3 we show the relationships between the various hierarchies of inner approximations for COP_n . Section 4 is devoted to the proof of Theorem 2.3. We conclude with some final remarks in Section 5.

Notation

Set $[n] = \{1, \dots, n\}$, and let \mathcal{D}^n denote the set of diagonal matrices and \mathcal{D}_{++}^n the set of diagonal matrices with positive diagonal entries. For $d \in \mathbb{R}^n$ we let $D = \text{Diag}(d) \in \mathcal{D}^n$ denote the diagonal matrix with diagonal entries $D_{ii} = d_i$ for $i \in [n]$. For $x \in \mathbb{R}^n$, $\|x\| = \sqrt{\sum_{i=1}^n x_i^2}$ denotes its Euclidean norm and $\|x\|_1 = \sum_{i=1}^n |x_i|$ denotes its ℓ_1 -norm. For a vector $x \in \mathbb{R}^n$, $\text{Supp}(x) = \{i \in [n] : x_i \neq 0\}$ denotes its support. The vectors e_1, \dots, e_n denote the standard basis vectors in \mathbb{R}^n , and $e = e_1 + \dots + e_n$ is the all-ones vector.

Given polynomials p_1, \dots, p_k , we let $(p_1, \dots, p_k) = \{\sum_{i=1}^k u_i p_i : u_i \in \mathbb{R}[x]\}$ denote the ideal generated by the p_i 's. Throughout we denote by I_Δ the ideal generated by the polynomial $\sum_{i=1}^n x_i - 1$. For a subset $S \subseteq [n]$ and variables $x = (x_1, \dots, x_n)$, we use the notation $x^S = \prod_{i \in S} x_i$ and, for a sequence $\beta \in \mathbb{N}^n$, we set $x^\beta = x_1^{\beta_1} \dots x_n^{\beta_n}$.

2. Overview of results and methods

In this section we give a broad overview of the strategy that we will follow to show our main result. As indicated above, we need to show that every positive diagonal scaling of the special matrices $T(\psi)$ (introduced below in relation (2.7)) lies in some cone $\mathcal{K}_5^{(r)}$. In fact we will show a sharper result and show membership in another, more restricted, conic hierarchy. This alternative conic hierarchy arises naturally by considering other sufficient positivity conditions for the polynomials $x^T M x$ and $(x^{\circ 2})^T M x^{\circ 2}$. We begin with introducing these alternative conic approximations.

2.1. Alternative conic approximations for COP_n

The definitions of the cone COP_n in (1.1) and in (1.2) rely on requiring, respectively, nonnegativity of the polynomial $x^T M x$ on \mathbb{R}_+^n , and nonnegativity of the polynomial $(x^{\circ 2})^T M x^{\circ 2}$ on \mathbb{R}^n . Since these two polynomials are homogeneous, this is equivalent to requiring, respectively, nonnegativity of $x^T M x$ on the standard simplex $\Delta_n = \{x \in \mathbb{R}_+^n : \sum_{i=1}^n x_i = 1\}$, and nonnegativity of $(x^{\circ 2})^T M x^{\circ 2}$ on the unit sphere $\mathbb{S}^{n-1} = \{x \in \mathbb{R}^n : \sum_{i=1}^n x_i^2 = 1\}$. In other words we can reformulate the copositive cone as

$$\text{COP}_n = \{M \in \mathcal{S}^n : x^T M x \geq 0 \text{ for all } x \in \Delta_n\}, \quad (2.1)$$

$$\text{COP}_n = \{M \in \mathcal{S}^n : (x^{\circ 2})^T M x^{\circ 2} \geq 0 \text{ for all } x \in \mathbb{S}^{n-1}\}. \quad (2.2)$$

Now we relax the nonnegativity condition and ask instead for a sufficient condition for nonnegativity on the simplex Δ_n or on the unit sphere \mathbb{S}^{n-1} , in terms of sum-of-squares representations that involve the constraints defining the simplex or the sphere. This follows the commonly used approach in polynomial optimization, based on Lasserre-type relaxations (see [13] and overviews in, e.g., [14], [15]), which justifies our notation below.

For any integer $r \in \mathbb{N}$, based on definition (2.1) for COP_n , we define the following cones

$$\text{LAS}_{\Delta_n}^{(r)} = \left\{ M \in \mathcal{S}^n : x^T M x = \sigma_0 + \sum_{i=1}^n \sigma_i x_i + q \text{ for } \sigma_0 \in \Sigma_r, \sigma_i \in \Sigma_{r-1} \text{ and } q \in I_{\Delta} \right\}, \quad (2.3)$$

$$\text{LAS}_{\Delta_n, \text{P}}^{(r)} = \left\{ M \in \mathcal{S}^n : x^T M x = \sum_{S \subseteq [n], |S| \leq r} \sigma_S x^S + q \text{ for } \sigma_S \in \Sigma_{|S|-r} \text{ and } q \in I_{\Delta} \right\}. \quad (2.4)$$

Recall I_{Δ} is the ideal generated by $\sum_{i=1}^n x_i - 1$. The index ‘P’ used in the notation $\text{LAS}_{\Delta_n, \text{P}}^{(r)}$ refers to the fact that the decomposition uses the preordering, which consists of all conic combinations of products of the constraints defining the simplex with sum-of-squares polynomials as multipliers. Clearly, for any integer $r \geq 0$, we have

$$\text{LAS}_{\Delta_n}^{(r)} \subseteq \text{LAS}_{\Delta_n, \text{P}}^{(r)} \subseteq \text{COP}_n.$$

Moreover, the cones $\text{LAS}_{\Delta_n}^{(r)}$ cover the interior of the copositive cone.

Lemma 2.1. $\text{int}(\text{COP}_n) \subseteq \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}.$

This follows from Putinar’s Positivstellensatz [25] applied to the simplex (see Theorem 4.1).

In a similar manner, based on definition (2.2) for COP_n , we define the following cone

$$\text{LAS}_{\mathbb{S}^{n-1}}^{(r)} = \left\{ M \in \mathcal{S}^n : (x^{\odot 2})^T M x^{\odot 2} = \sigma_0 + u \left(\sum_{i=1}^n x_i^2 - 1 \right) \right. \\ \left. \text{for some } \sigma_0 \in \Sigma_r \text{ and } u \in \mathbb{R}[x] \right\}. \quad (2.5)$$

As we will show later (see Theorem 3.1), we have the following relationships between the various approximation cones for COP_n that were introduced above:

$$\text{LAS}_{\Delta_n}^{(r)} \subseteq \mathcal{K}_n^{(r-2)} = \text{LAS}_{\Delta_n, \text{P}}^{(r)} = \text{LAS}_{\mathbb{S}^{n-1}}^{(2r)} \quad \text{for any } n \geq 1 \text{ and } r \geq 2. \quad (2.6)$$

A main motivation for introducing the cones $\text{LAS}_{\Delta_n}^{(r)}$ lies in the fact that they permit to capture certain copositive matrices on the boundary of COP_n , namely those matrices M that arise as positive diagonal scaling of a class of matrices generating extreme rays of COP_5 (see Theorem 2.2 and Theorem 2.3 below). Of course, as a direct application of (2.6), these matrices also lie in some Parrilo cone $\mathcal{K}_n^{(r)}$. The point, however, is that we do not know how to show this directly, without showing that they belong to some cone $\text{LAS}_n^{(r)}$, which is a stronger result.

The alternative cones $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$ are introduced for the sake of completeness, since they arise naturally in view of definition (2.2) for COP_n , however we will not use them for the proofs of our results in the paper.

2.2. Extreme rays of COP_5

For answering the question of whether the two cones COP_5 and $\bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$ coincide it suffices to look at the matrices that generate an extreme ray of COP_5 . This indeed follows directly from the fact that any $M \in \text{COP}_5$ can be decomposed as a finite sum of matrices generating an extreme ray. For convenience we say that a copositive matrix is *extreme* if it generates an extreme ray of COP_n .

A *positive diagonal scaling* of a matrix M is a matrix of the form DMD where $D \in \mathcal{D}_{++}^n$. Notice that if M is an extreme matrix of COP_n then every positive diagonal scaling of M is also an extreme matrix. Moreover, if $M \in \text{COP}_n$ is an extreme matrix then the same holds for every row/column permutation of M , i.e., for any matrix of the form $P^T M P$, where P is a permutation matrix. As observed above, positive diagonal scaling does not preserve in general membership in $\mathcal{K}_n^{(r)}$ ($r \geq 1$), however taking a row/column permutation clearly does preserve membership in any $\mathcal{K}_n^{(r)}$ ($r \geq 0$).

Hildebrand [12] characterized the set of extreme matrices of COP_5 . For this, he defined the following matrices

$$T(\psi) = \begin{pmatrix} 1 & -\cos \psi_4 & \cos(\psi_4 + \psi_5) & \cos(\psi_2 + \psi_3) & -\cos \psi_3 \\ -\cos \psi_4 & 1 & -\cos \psi_5 & \cos(\psi_5 + \psi_1) & \cos(\psi_3 + \psi_4) \\ \cos(\psi_4 + \psi_5) & -\cos \psi_5 & 1 & -\cos \psi_1 & \cos(\psi_1 + \psi_2) \\ \cos(\psi_2 + \psi_3) & \cos(\psi_5 + \psi_1) & -\cos \psi_1 & 1 & -\cos \psi_2 \\ -\cos \psi_3 & \cos(\psi_3 + \psi_4) & \cos(\psi_1 + \psi_2) & -\cos \psi_2 & 1 \end{pmatrix}, \quad (2.7)$$

where $\psi \in \mathbb{R}^5$, and proved the following theorem.

Theorem 2.2 ([12]). *Let $M \in \text{COP}_5$ be an extreme matrix, and assume that M is neither an element of $\mathcal{K}_5^{(0)}$ nor a positive diagonal scaling (of a row/column permutation) of the Horn matrix. Then M is of the form*

$$M = P \cdot D \cdot T(\psi) \cdot D \cdot P^T,$$

where P is a permutation matrix, $D \in \mathcal{D}_{++}^5$ and the quintuple ψ is an element of the set

$$\Psi = \left\{ \psi \in \mathbb{R}^5 : \sum_{i=1}^5 \psi_i < \pi, \psi_i > 0 \text{ for } i \in [5] \right\}. \quad (2.8)$$

In summary, the extreme matrices M of COP_5 can be divided into three categories:

- (i) $M \in \mathcal{K}_5^{(0)}$,
- (ii) M is (up to row/column permutation) a positive diagonal scaling of the Horn matrix,
- (iii) M is (up to row/column permutation) a positive diagonal scaling of a matrix $T(\psi)$ for some $\psi \in \Psi$.

Our main result in this paper is to show that every matrix from the third category of extreme matrices of COP_5 belongs to some cone $\text{LAS}_{\Delta_5}^{(r)}$ and thus, in view of (2.6), to some cone $\mathcal{K}_5^{(r)}$.

Theorem 2.3. *Let $D \in \mathcal{D}_{++}^5$ be a positive diagonal matrix. Then, for all $\psi \in \Psi$, we have $D \cdot T(\psi) \cdot D \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_5}^{(r)} \subseteq \bigcup_{r \geq 0} \mathcal{K}_5^{(r)}$.*

In view of Theorem 2.2, Theorem 1.3 directly follows from Theorem 2.3. As a direct consequence, in order to answer Question 1.1, it suffices to look at the extreme matrices from the second category (i.e., at the positive diagonal scalings of the Horn matrix H).

On the other hand, as we will show later in Lemma 3.10, the Horn matrix H does not belong to any of the cones $\text{LAS}_{\Delta_5}^{(r)}$. Hence, in order to show that any diagonal scaling of the Horn matrix belongs to some cone $\mathcal{K}_5^{(r)}$ and thus give an affirmative answer to Question 1.1, it will not be sufficient to consider the cones $\text{LAS}_{\Delta_5}^{(r)}$. A different, new strategy will be needed.

2.3. Sketch of the proof

We are left with the task of proving Theorem 2.3. For this we follow an optimization approach and consider the following standard quadratic program, for a given copositive matrix $M \in \text{COP}_n$:

$$p_M^* := \min\{x^T M x : x \in \Delta_n\}. \quad (\text{SQP}_M)$$

If $p_M^* > 0$ then $M \in \text{int}(\text{COP}_n)$ and thus, by Lemma 2.1, $M \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$. Hence we may restrict our attention to the case when $p_M^* = 0$, i.e., when $M \in \partial \text{COP}_n$. We now consider the Lasserre sum-of-squares hierarchy for problem (SQP_M) , where, for any integer $r \geq 1$, we set

$$p_M^{(r)} := \sup\{\lambda : x^T M x - \lambda = \sigma_0 + \sum_{i=1}^n x_i \sigma_i + q \text{ for some } q \in I_\Delta, \text{ and } \sigma_0 \in \Sigma_r, \sigma_i \in \Sigma_{r-1}\}. \quad (2.9)$$

Then the bounds $p_M^{(r)}$ converge asymptotically to $p_M^* = 0$. Moreover, in program (2.9) the supremum is attained and thus one may replace ‘sup’ by ‘max’. Hence, we have $p_M^{(r)} = 0$ if and only if the matrix M belongs to the cone $\text{LAS}_n^{(r)}$. Therefore, when $p_M^* = 0$, we have $M \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ if and only if the Lasserre hierarchy (2.9) has finite convergence, i.e., $p_M^{(r)} = 0$ for some r . Based on this observation, our strategy is now to show finite convergence of the Lasserre hierarchy (2.9) in the case when M is a positive diagonal scaling of a matrix $T(\psi)$ with $\psi \in \Psi$.

For this we will use a general theorem of Nie [21] that ensures finite convergence of the Lasserre hierarchy (2.9) when the classical optimality conditions hold at every global minimizer (see Theorem 4.2 below). In our case the global minimizers of problem (SQP_M) are given by the zeros of the quadratic form $x^T M x$ in Δ_n , whose structure is well-understood for the matrices $M = T(\psi)$. See Section 4 for details.

3. Relationships between sum-of-squares conic approximations for COP_n

In this section we show the relationships from (2.6) between the cones $\mathcal{K}_n^{(r)}$, $\text{LAS}_{\Delta_n}^{(r)}$, $\text{LAS}_{\Delta_n, P}^{(r)}$ and $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$ introduced in the previous sections. In addition, we highlight the relationship to the cones $\mathcal{Q}_n^{(r)}$ introduced in [23] and point out how these cones can all be seen as distinct variations within a common framework.

3.1. Links between the cones $\mathcal{K}_n^{(r)}$, $\text{LAS}_{\Delta_n}^{(r)}$, $\text{LAS}_{\Delta_n, P}^{(r)}$, and $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$

Here we show the following result, which establishes the links announced in relation (2.6) between the various cones defined in previous sections. This result is implicitly shown in [16] (see Corollary 3.9), where we compared different bounds for standard quadratic programs obtained via sums of squares of polynomials.

Theorem 3.1. *Let $r \geq 2$ and $n \geq 1$, then we have*

$$\text{LAS}_{\Delta_n}^{(r)} \subseteq \mathcal{K}_n^{(r-2)} = \text{LAS}_{\Delta_n, P}^{(r)} = \text{LAS}_{\mathbb{S}_{n-1}}^{(2r)}.$$

We begin with observing that in the definition (2.4) of the cone $\text{LAS}_{\Delta_n, P}^{(r)}$ we may assume that the summation only involves sets $S \subseteq [n]$ with $|S| \equiv r \pmod{2}$.

Lemma 3.2. *We have*

$$\text{LAS}_{\Delta_n, P}^{(r)} = \left\{ M \in \mathcal{S}^n : x^T M x = \sum_{\substack{S \subseteq [n], |S| \leq r \\ |S| \equiv r \pmod{2}}} \sigma_S x^S + q \text{ with } \sigma_S \in \Sigma_{r-|S|} \text{ and } q \in I_\Delta \right\}.$$

Proof. To see this consider a term $x^S \sigma_S$, where $|S| \leq r$, $|S| \not\equiv r \pmod{2}$ and $\sigma_S \in \Sigma_{r-|S|}$. Then $|S| \leq r-1$, $\deg(\sigma_S) \leq r-|S|-1$ and thus, modulo the ideal I_Δ , we can replace $x^S \sigma_S$ by $x^S \sigma_S(\sum_{i=1}^n x_i)$. Now expand this expression as $\sum_{i \in S} x^{S \setminus \{i\}} \cdot \sigma_S x_i^2 + \sum_{i \in [n] \setminus S} x^{S \cup \{i\}} \sigma_S$. So each term in this summation is of the form $x^T \sigma_T$ with $|T| \leq r$, $|T| \equiv r \pmod{2}$, and $\deg(\sigma_T) \leq r - |T|$. \square

Next we recall an alternative definition of the cone $\mathcal{K}_n^{(r)}$, following from a result in [27].

Theorem 3.3 ([27], Prop 9). *Let $f \in \mathbb{R}[x]$ be a homogeneous polynomial with $\deg(f) = d$. Then the polynomial $f(x^2)$ is a sum of squares if and only if f admits a decomposition of the form*

$$f = \sum_{\substack{S \subseteq [n], |S| \leq d \\ |S| \equiv d \pmod{2}}} \sigma_S x^S \text{ for some } \sigma_S \in \Sigma_{d-|S|}. \quad (3.1)$$

In particular, for any $r \geq 0$, we have

$$\mathcal{K}_n^{(r)} = \left\{ M \in \mathcal{S}^n : \left(\sum_{i=1}^n x_i \right)^r x^T M x = \sum_{\substack{S \subseteq [n], |S| \leq r+2 \\ |S| \equiv r \pmod{2}}} \sigma_S x^S \text{ for some } \sigma_S \in \Sigma_{r+2-|S|} \right\}. \quad (3.2)$$

Note the similarity between the description of $\text{LAS}_{\Delta_n, P}^{(r)}$ in Lemma 3.2 and that of $\mathcal{K}_n^{(r-2)}$ in relation (3.2). The difference lies in the fact that for $\text{LAS}_{\Delta_n, P}^{(r)}$ we have a representation of $x^T M x$ modulo the ideal I_Δ , while for $\mathcal{K}_n^{(r-2)}$ we have a representation of $(\sum_i x_i)^{r-2} x^T M x$. The next lemma (whose main idea was already used, e.g., in [9]) gives a simple trick, useful to navigate between these two types of representations.

Lemma 3.4. *Let $f, g \in \mathbb{R}[x]$ and assume f is homogeneous. The following assertions hold.*

- (i) If $(\sum_{i=1}^n x_i)^r f(x) = g(x)$, then $f - g \in I_\Delta$.
 (ii) Let $\deg(f) = d$, $\deg(g) = d + r$ ($r \in \mathbb{N}$), and define $\tilde{g}(x) = (\sum_{i=1}^n x_i)^{d+r} g(x / (\sum_{i=1}^n x_i))$. Then, \tilde{g} is a homogeneous polynomial of degree $d+r$. Moreover, if $f - g \in I_\Delta$, then $(\sum_{i=1}^n x_i)^r f(x) = \tilde{g}(x)$.

Proof. The assertion (i) follows by expanding $(\sum_{i=1}^n x_i)^r$ as the sum

$$\left(\sum_{i=1}^n x_i\right)^r = \left(\sum_{i=1}^n x_i - 1 + 1\right)^r = 1 + \left(\sum_{i=1}^n x_i - 1\right) \left(\sum_{k=1}^r \binom{r}{k} \left(\sum_{i=1}^n x_i - 1\right)^{k-1}\right).$$

We now show (ii). The claim that \tilde{g} is a homogeneous polynomial of degree $d + r$ is easy to check. Assume now $f - g \in I_\Delta$. By evaluating $f - g$ at $x / (\sum_{i=1}^n x_i)$, we obtain $f(x / (\sum_{i=1}^n x_i)) = g(x / (\sum_{i=1}^n x_i))$. As f is homogeneous of degree d this implies $f(x) = (\sum_{i=1}^n x_i)^d g(x / (\sum_{i=1}^n x_i))$, and the result follows after multiplying both sides by $(\sum_{i=1}^n x_i)^r$. \square

We will also use the following simple fact.

Lemma 3.5. Let $\sigma \in \Sigma_k$ and define $\tilde{\sigma}(x) = (\sum_{i=1}^n x_i)^k \sigma(x / (\sum_{i=1}^n x_i))$. Then $\tilde{\sigma}$ is a homogeneous polynomial of degree k . Moreover,

- (i) If $k \equiv \deg(\sigma) \pmod{2}$, then $\tilde{\sigma} \in \Sigma$.
 (ii) If $k \not\equiv \deg(\sigma) \pmod{2}$, then $\tilde{\sigma} = (\sum_{i=1}^n x_i) \hat{\sigma}$, where $\hat{\sigma} \in \Sigma$.

Proof. Note that $\tilde{\sigma} = (\sum_{i=1}^n x_i)^{k-\deg(\sigma)} \sigma'$, where $\sigma' := (\sum_{i=1}^n x_i)^{\deg(\sigma)} \sigma(x / (\sum_{i=1}^n x_i))$ is a homogeneous polynomial with degree $\deg(\sigma)$. It suffices now to observe that $(\sum_{i=1}^n x_i)^{k-\deg(\sigma)}$ is a square if $k - \deg(\sigma)$ is even, and it is a square times $(\sum_i x_i)$ if $k - \deg(\sigma)$ is odd. \square

Using these two lemmas we can now relate the two cones $\text{LAS}_{\Delta_n, P}^{(r)}$ and $\mathcal{K}_n^{(r-2)}$.

Lemma 3.6. For any $r \geq 2$, we have $\text{LAS}_{\Delta_n, P}^{(r)} = \mathcal{K}_n^{(r-2)}$.

Proof. First assume $M \in \text{LAS}_{\Delta_n, P}^{(r)}$. Using Lemma 3.2, we have a decomposition of the form $x^T M x = g(x) + q(x)$, where $q \in I_\Delta$ and $g(x) = \sum_{|S| \leq r, |S| \equiv r \pmod{2}} \sigma_S x^S$, with $\sigma_S \in \Sigma_{r-|S|}$. Using Lemma 3.4(ii) we get

$$\begin{aligned} \left(\sum_{i=1}^n x_i\right)^{r-2} x^T M x &= \left(\sum_{i=1}^n x_i\right)^r g\left(\frac{x}{\sum_i x_i}\right) \\ &= \sum_{|S| \leq r, |S| \equiv r \pmod{2}} x^S \underbrace{\left(\sum_{i=1}^n x_i\right)^{r-|S|} \sigma_S\left(\frac{x}{\sum_i x_i}\right)}_{=\tilde{\sigma}_S(x)}. \end{aligned}$$

As $r - |S| \equiv \deg(\tilde{\sigma}_S) \pmod{2}$ we have $\tilde{\sigma}_S \in \Sigma_{r-|S|}$ by Lemma 3.5(i). In view of relation (3.2), this shows that $M \in \mathcal{K}_n^{(r-2)}$.

Conversely, assume $M \in \mathcal{K}_n^{(r-2)}$. Then, in view of (3.2), we have a decomposition of the form $(\sum_{i=1}^n x_i^2)^{r-2} x^T M x = \sum_{|S| \leq r, |S| \equiv r \pmod{2}} \sigma_S x^S$, where $\sigma_S \in \Sigma_{r-|S|}$. By applying Lemma 3.4(i), we obtain $x^T M x = \sum_{|S| \leq r, |S| \equiv r \pmod{2}} \sigma_S x^S + q$, where $q \in I_\Delta$. Combining with Lemma 3.2 this shows $M \in \text{LAS}_{\Delta_n, P}^{(r)}$. \square

To complete the proof of Theorem 3.1 we now establish the relation to the cone $\text{LAS}_{\mathbb{S}^{n-1}}^{(r)}$, which follows from a result in [9].

Proposition 3.7 ([9]). *Let f be a homogeneous polynomial of degree $2d$ and $r \in \mathbb{N}$. Then, $f\left(\sum_{i=1}^n x_i^2\right)^r \in \Sigma$ if and only if $f = \sigma + u(\sum_{i=1}^n x_i^2 - 1)$ for some $\sigma \in \Sigma_{2r+2d}$ and $u \in \mathbb{R}[x]$.*

In particular, for any $r \geq 2$ we have

$$\text{LAS}_{\mathbb{S}^{n-1}}^{(r)} = \left\{ M \in \mathcal{S}^n : \left(\sum_{i=1}^n x_i^2 \right)^{r-2} (x^{\circ 2})^T M x^{\circ 2} \in \Sigma \right\} = \mathcal{K}_n^{(r-2)}. \quad (3.3)$$

We conclude this section with a reformulation for the cone $\text{LAS}_{\Delta_n}^{(r)}$ in the same vein as the reformulation of $\text{LAS}_{\Delta_n, P}^{(r)}$ in Lemma 3.2.

Lemma 3.8. *Let $r \geq 2$. If r is odd, then we have*

$$\text{LAS}_{\Delta_n}^{(r)} = \left\{ M \in \mathcal{S}^n : \left(\sum_{i=1}^n x_i \right)^{r-2} x^T M x = \sum_{i=1}^n \sigma_i x_i \text{ with } \sigma_i \in \Sigma_{r-1} \right\}. \quad (3.4)$$

If r is even and $r \geq 4$, then we have $\text{LAS}_{\Delta_n}^{(r)} = \text{LAS}_{\Delta_n}^{(r-1)}$.

Proof. The proof is similar to that of Lemma 3.2, except we now have a summation that involves only sets $S \subseteq [n]$ with $|S| \leq 1$. We spell out the details for clarity. Consider first the case when r is odd. Assume $M \in \text{LAS}_{\Delta_n}^{(r)}$, so that $x^T M x = \sigma_0 + \sum_{i=1}^n \sigma_i x_i + q$, where $q \in I_\Delta, \sigma_0 \in \Sigma_r, \sigma_i \in \Sigma_{r-1}$. Combining Lemma 3.4(ii) and Lemma 3.5 we obtain a decomposition as in (3.4). Conversely, starting from a decomposition as in (3.4) we get a decomposition as in (2.3) by applying Lemma 3.4(i).

Consider now the case $r \geq 4$ even. Assume $M \in \text{LAS}_{\Delta_n}^{(r)}$, we show $M \in \text{LAS}_{\Delta_n}^{(r-1)}$. Starting from a decomposition as in (2.3) and using as above Lemma 3.4(i) and Lemma 3.5, we obtain a decomposition

$$\left(\sum_{j=1}^n x_j \right)^{r-2} x^T M x = \tilde{\sigma}_0 + \left(\sum_{j=1}^n x_j \right) \sum_{i=1}^n \tilde{\sigma}_i x_i,$$

where $\tilde{\sigma}_0 \in \Sigma_r$ and $\tilde{\sigma}_i \in \Delta_{r-1}$. From this it follows that the polynomial $\sum_{j=1}^n x_j$ divides $\tilde{\sigma}_0$, which implies its square divides $\tilde{\sigma}_0$. Then we can divide out by $\sum_{j=1}^n x_j$ and obtain an expression as in (3.4) (replacing r by $r - 1$), that certifies membership of M in $\text{LAS}_{\Delta_n}^{(r-1)}$. \square

3.2. Link to the cones $\mathcal{Q}_n^{(r)}$

The definition (3.2) of the cone $\mathcal{K}_n^{(r)}$ involves only square-free monomials, of the form $x^S = \prod_{i \in S} x_i$. As observed in [27,23], one can allow arbitrary monomials and, after using again the argument of Lemma 3.4, we get the following alternative definitions

$$\begin{aligned} \mathcal{K}_n^{(r)} &= \left\{ M \in \mathcal{S}^n : \left(\sum_{i=1}^n x_i \right)^r x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta| \leq r+2}} \sigma_\beta x^\beta \text{ for } \sigma_\beta \in \Sigma_{r+2-|\beta|} \right\} \quad (3.5) \\ &= \left\{ M \in \mathcal{S}^n : x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta| \leq r+2}} \sigma_\beta x^\beta + q \text{ for } \sigma_\beta \in \Sigma_{r+2-|\beta|} \text{ and } q \in I_\Delta \right\}. \quad (3.6) \end{aligned}$$

Based on relation (3.5), the authors of [23] proposed the cones $\mathcal{Q}_n^{(r)}$, that are defined as the variation (3.7) of (3.5) obtained by just considering the terms associated to the monomials x^β with highest degree r or $r + 2$. In other words,

$$\begin{aligned} \mathcal{Q}_n^{(r)} &= \left\{ M \in \mathcal{S}^n : \left(\sum_{i=1}^n x_i \right)^r x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta|=r, r+2}} \sigma_\beta x^\beta \text{ for } \sigma_\beta \in \Sigma_{r+2-|\beta|} \right\}, \quad (3.7) \\ &= \left\{ M \in \mathcal{S}^n : x^T M x = \sum_{\substack{\beta \in \mathbb{N}^n \\ |\beta|=r, r+2}} \sigma_\beta x^\beta + q \text{ for } \sigma_\beta \in \Sigma_{r+2-|\beta|} \text{ and } q \in I_\Delta \right\}, \quad (3.8) \end{aligned}$$

where the equivalence of (3.7) and (3.8) follows again using Lemma 3.4. Clearly, we have inclusion $\mathcal{Q}_n^{(r)} \subseteq \mathcal{K}_n^{(r)}$ for all $n \geq 1$ and $r \geq 0$, with equality $\mathcal{Q}_n^{(r)} = \mathcal{K}_n^{(r)}$ for $r = 0, 1$.

Remark 3.9. For any $r \geq 2$, the two cones $\text{LAS}_{\Delta_n}^{(r)}$ and $\mathcal{Q}_n^{(r-2)}$ are both contained in the cone $\mathcal{K}_n^{(r-2)}$. In view of (3.6), membership in $\mathcal{K}_n^{(r-2)}$ requires a decomposition using terms of the form $x^\beta \sigma_\beta$ for all β such that $|\beta| \leq r$ and $|\beta| \equiv r \pmod{2}$. In view of (2.3), for membership in $\text{LAS}_{\Delta_n}^{(r)}$, we consider only the terms $x^\beta \sigma_\beta$ with lowest degree $|\beta| = 0, 1$. On the other hand, in view of (3.8), for membership in $\mathcal{Q}_n^{(r-2)}$, we consider only the terms with highest degree $|\beta| = r, r - 2$. Hence, it is interesting to note that the two cones $\text{LAS}_{\Delta_n}^{(r)}$ and $\mathcal{Q}_n^{(r-2)}$ use the “two opposite ends” of the spectrum of possible degrees for the terms $x^\beta \sigma_\beta$.

We conclude this section with observing that, while the Horn matrix H belongs to $\mathcal{K}_5^{(1)}$, it in fact does not belong to any of the cones $\text{LAS}_{\Delta_n}^{(r)}$. The proof exploits the fact that the quadratic form $x^T H x$ has infinitely many zeros in the simplex Δ_n .

Lemma 3.10. *For all $r \in \mathbb{N}$ we have $H \notin \text{LAS}_{\Delta_5}^{(r)}$.*

Proof. Assume by contradiction that $H \in \text{LAS}_{\Delta_5}^{(r)}$ for some $r \in \mathbb{N}$, i.e.,

$$x^T H x = \sigma_0 + \sum_{i=1}^5 x_i \sigma_i + q(x) \left(\sum_{i=1}^5 x_i - 1 \right),$$

for some $\sigma_0, \sigma_i \in \Sigma$ and $q(x) \in \mathbb{R}[x]$. For a fixed scalar $t \in (0, 1)$, consider the vector $u_t = (\frac{1}{2}, 0, \frac{t}{2}, \frac{1-t}{2}, 0) \in \Delta_5$, which can be verified to define a zero of $x^T H x$, i.e., $u_t^T H u_t = 0$. By evaluating the quadratic form $x^T H x$ at the point $x + u_t$ we obtain

$$(x + u_t)^T H (x + u_t) = \sigma_0(x + u_t) + \sum_{i=1}^5 (x + u_t)_i \sigma_i(x + u_t) + q(x + u_t) \left(\sum_{i=1}^5 x_i \right).$$

As $u_t^T H u_t = 0$ and $x^T H u_t = x_2 t + (1 - t)x_5$ we obtain

$$\begin{aligned} x^T H x + 2x_2 t + 2(1 - t)x_5 &= \sigma_0(x + u_t) + \frac{1}{2}\sigma_1(x + u_t) + \frac{t}{2}\sigma_3(x + u_t) + \frac{1-t}{2}\sigma_4(x + u_t) \\ &\quad + \sum_{i=1}^5 x_i \sigma_i(x + u_t) + q(x + u_t) \left(\sum_{i=1}^5 x_i \right). \end{aligned} \tag{3.9}$$

We now compare some coefficients of the monomials (in x) in both sides of (3.9) in order to reach a contradiction. As there is no constant term in the left hand side, the constant term in the right hand side is equal to 0. This gives $\sigma_0(u_t) + \sigma_1(u_t)/2 + t\sigma_3(u_t)/2 + (1 - t)\sigma_4(u_t) = 0$ and thus $\sigma_i(u_t) = 0$ for $i = 0, 1, 3, 4$. As $\sigma_i(x + u_t)$ is a sum-of-squares polynomial in x this in turn implies that there is no linear term in x in each of the polynomials $\sigma_i(x + u_t)$ for $i = 0, 1, 3, 4$. Next, combining this with the fact that the coefficient of x_1 in the left hand side is equal to 0, one obtains that the polynomial $q(x + u_t)$ has no constant term (i.e., $q(u_t) = 0$). Now we compare the coefficients of x_2 in both sides. In the left hand side it is equal to $2t$, while in the right hand side it is equal to $\sigma_2(u_t)$. Hence we have $2t = \sigma_2(u_t)$. We now reach a contradiction since $\sigma_2(u_t)$ is a sum-of-squares polynomial in t . \square

We now show that the cones $\text{LAS}_{\Delta_n}^{(r)}$ cover the copositive cone only in the case $n = 2$.

Proposition 3.11. *We have $\text{COP}_2 = \text{LAS}_{\Delta_2}^{(3)}$, and the inclusion $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)} \subset \text{COP}_n$ is strict for any $n \geq 3$.*

Proof. First, assume $M = \begin{pmatrix} a & c \\ c & b \end{pmatrix} \in \text{COP}_2$, we show $M \in \text{LAS}_{\Delta_2}^{(3)}$. Note that $a, b \geq 0$ and $c \geq -\sqrt{ab}$ (using the fact that $u^T M u \geq 0$ with $u = (1, 0)$, $(0, 1)$, and (\sqrt{b}, \sqrt{a})). Then we can write $x^T M x = (\sqrt{a}x_1 - \sqrt{b}x_2)^2 + 2(c + \sqrt{ab})x_1x_2$, which, modulo the ideal I_Δ , is equal to $(\sqrt{a}x_1 - \sqrt{b}x_2)^2(x_1 + x_2) + 2(c + \sqrt{ab})(x_2^2x_1 + x_1^2x_2)$, thus showing $M \in \text{LAS}_{\Delta_2}^{(3)}$.

Assume now $n = 3$, we show that the matrix

$$M = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \in \text{COP}_3$$

does not belong to any of the cones $\text{LAS}_{\Delta_3}^{(r)}$. The proof follows a similar argument as the one used for Lemma 3.10, using the fact that $u_t = (t, 0, 1 - t)$ defines a zero of M for any $t \in (0, 1)$, i.e., $u_t^T M u_t = 0$. \square

4. Proof of Theorem 2.3

We now proceed to prove Theorem 2.3. As mentioned in Section 2.3, we will follow an optimization approach, which allows us to apply a result of Nie [21] as a key ingredient for our proof. We proceed in three steps. First, we recall the sum-of-squares Lasserre hierarchy for a general polynomial optimization problem and the result of Nie [21], that shows finite convergence of this hierarchy under the classical optimality conditions. Second, applying this result to a class of standard quadratic programs, we obtain a set of sufficient conditions for a matrix $M \in \partial\text{COP}_n$, that permit to claim that every positive diagonal scaling of M belongs to some cone $\text{LAS}_{\Delta_n}^{(r)}$. Finally, we show that these sufficient conditions hold for the matrices $T(\psi)$ ($\psi \in \Psi$), which concludes the proof of Theorem 2.3.

4.1. Optimality conditions and finite convergence of Lasserre hierarchy

In this section we recall a useful general result of Nie [21] that gives sufficient conditions for having finite convergence of the Lasserre hierarchy for a general polynomial optimization problem.

Given n -variate polynomials f, g_j for $j \in [m]$, and h_i for $i \in [k]$, consider the general polynomial optimization problem

$$f_{\min} = \inf_{x \in K} f(x), \quad (\text{Poly-Opt})$$

where K is the semialgebraic set defined by

$$K = \{x \in \mathbb{R}^n : g_j(x) \geq 0 \text{ for } j \in [m], h_i(x) = 0 \text{ for } i \in [k]\}.$$

We say that the *Archimedean condition* holds if there exists $N \in \mathbb{R}$ such that

$$N - \sum_{i=1}^n x_i^2 = \sigma_0 + \sum_{j=1}^m \sigma_j g_j + \sum_{i=1}^k u_i h_i \quad \text{for some } \sigma_0, \sigma_j \in \Sigma \text{ and } u_i \in \mathbb{R}[x]. \quad (4.1)$$

For any integer $r \in \mathbb{N}$ consider the corresponding Lasserre sum-of-squares hierarchy

$$f^{(r)} = \sup \left\{ \lambda : f - \lambda = \sigma_0 + \sum_{j=1}^m \sigma_j g_j + \sum_{i=1}^k u_i h_i(x) \text{ for some } \sigma_0 \in \Sigma_r, \sigma_i \in \Sigma_{r-\deg(g_i)} \right. \\ \left. \text{and } u_i \in \mathbb{R}[x]_{r-\deg(h_i)} \right\}. \quad (4.2)$$

By the following result of Putinar [25], under the Archimedean condition, asymptotic convergence is guaranteed, i.e., $f^{(r)} \rightarrow f_{\min}$ as $r \rightarrow \infty$.

Theorem 4.1 ([25]). *Assume \mathcal{K} satisfies the Archimedean condition (4.1). If a polynomial p is strictly positive on K , then p can be written as $p = \sigma_0 + \sum_{j=1}^m \sigma_j g_j + \sum_{i=1}^k u_i h_i$ for some $\sigma_0, \sigma_j \in \Sigma$ ($j \in [m]$) and $u_i \in \mathbb{R}[x]$ ($i \in [k]$).*

The Lasserre hierarchy is said to have *finite convergence* if $f^{(r)} = f_{\min}$ for some $r \in \mathbb{N}$. In general, finite convergence is not always achieved. However, Nie showed in [21] a very useful result that permits to show finite convergence of the Lasserre hierarchy under some extra conditions apart from the Archimedean condition. These conditions rely on the classical optimality conditions, that we now recall (see, e.g., the textbook [1]).

Let u be a local minimizer of problem (Poly-Opt) and let $J(u) = \{j \in [m] : g_j(u) = 0\}$ be the set of inequality constraints that are active at u . Then the *constraint qualification constraint* (abbreviated as CQC) holds at u if the set $\{\nabla g_j(u) : j \in J(u)\} \cup \{\nabla h_i(u) : i \in [k]\}$ is linearly independent. If CQC holds at u then there exist scalars $\lambda_1, \dots, \lambda_k, \mu_1, \dots, \mu_m \in \mathbb{R}$ satisfying

$$\nabla f(u) = \sum_{i=1}^k \lambda_i \nabla h_i(u) + \sum_{j \in J(u)} \mu_j \nabla g_j(u), \\ \mu_j \geq 0 \text{ for } j \in J(u), \quad \mu_j = 0 \text{ for } j \in [m] \setminus J(u).$$

If, in addition, $\mu_j > 0$ holds for all $j \in J(u)$, then one says that the *strict complementarity condition* (abbreviated as SCC) holds. Let $L(x)$ the Lagrangian function, defined by

$$L(x) = f(x) - \sum_{i=1}^k \lambda_i h_i(x) - \sum_{j \in J(u)} \mu_j g_j(x).$$

Another necessary condition for u to be a local minimizer is the following inequality

$$v^T \nabla^2 L(u) v \geq 0 \text{ for all } v \in G(u)^\perp, \quad (\text{SONC})$$

where $G(u)$ is defined by

$$G(u)^\perp = \{x \in \mathbb{R}^n : x^T \nabla g_j(u) = 0 \text{ for all } j \in J(u) \text{ and } x^T \nabla h_i(u) = 0 \text{ for all } i \in [k]\}.$$

If it happens that the inequality (SONC) is strict, i.e., if

$$v^T \nabla^2 L(u) v > 0 \text{ for all } 0 \neq v \in G(u)^\perp, \quad (\text{SOSC})$$

then one says that the *second order sufficiency condition* (SOSC) holds at u .

We can now state the following result by Nie [21].

Theorem 4.2 ([21]). *Assume the Archimedean condition (4.1) holds for the polynomial tuples h and g in problem (Poly-Opt). If the constraint qualification condition (CQC), the strict complementarity condition (SCC), and the second order sufficiency condition (SOSC) hold at every global minimizer of (Poly-Opt), then the Lasserre hierarchy (4.2) has finite convergence, i.e., $f^{(r)} = f_{\min}$ for some $r \in \mathbb{N}$.*

In the next section we will apply Theorem 4.2 to a class of standard quadratic programs in order to show finite convergence of the corresponding Lasserre hierarchy. One important observation, already made in [21], is that this strategy can only work when the number of global minimizers is finite.

4.2. Optimality conditions for standard quadratic programs

Consider a matrix $M \in \partial\text{COP}_n$. The objective of this section is to give sufficient conditions on M that permit to conclude that $DMD \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ for all $D \in \mathcal{D}_{++}^n$. This will be very useful since, in the next section, we will show that the matrices $T(\psi)$ ($\psi \in \Psi$) satisfy these sufficient conditions and thus we will be able to conclude the proof of Theorem 2.3. Our strategy is to apply the result from Theorem 4.2 to the setting of standard quadratic programs. Let us recall the following problem, already introduced in Section 2.3:

$$\min\{x^T M x : x \in \Delta_n\} \quad (\text{SQP}_M)$$

and the corresponding Lasserre hierarchy introduced in relation (2.9). Note the optimal value of (SQP_M) is zero as $M \in \partial\text{COP}_n$.

Now we will apply Theorem 4.2 to problem (SQP_M). The set $K = \Delta_n$ indeed satisfies the Archimedean condition (this is well-known and easy to check; see, e.g., [16]). By [18, Theorem 3.1], the feasible region of the Lasserre hierarchy (2.9) associated to problem (SQP_M) is a closed set. Hence, the ‘sup’ in program (2.9) can be changed to a ‘max’. As a consequence, for a matrix $M \in \partial\text{COP}_n$, having finite convergence of the Lasserre hierarchy (2.9) associated to problem (SQP_M) is equivalent to having $M \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$. So we obtain the following corollary.

Corollary 4.3. *Let $M \in \partial\text{COP}_n$. If the optimality conditions (CQC), (SCC) and (SOSC) hold at every global minimizer of problem (SQP_M) then $M \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$.*

As mentioned earlier, our objective is to give sufficient conditions on M that permit to claim $DMD \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ for all $D \in \mathcal{D}_{++}^n$. For this we will apply Corollary 4.3, combined with the following result, which will be a key ingredient in our argument.

Theorem 4.4. *If the optimality conditions hold at every minimizer of problem (SQP_M) for a matrix $M \in \partial\text{COP}_n$, then, for every $D \in \mathcal{D}_{++}^n$, they also hold at every minimizer of problem (SQP_{DMD}) .*

In what follows we will prove Theorem 4.4. Given $M \in \partial\text{COP}_n$ and $D \in \mathcal{D}_{++}^n$, let us consider the standard quadratic program associated to DMD :

$$\min\{x^T DMDx : x \in \Delta_n\}. \quad (\text{SQP}_{DMD})$$

Observe that the optimal value of program (SQP_{DMD}) is zero. Indeed, if $u \in \Delta_n$ is a minimizer of problem (SQP_M) , then $\frac{D^{-1}u}{\|D^{-1}u\|_1} \in \Delta_n$ is a minimizer of problem (SQP_{DMD}) . Conversely, if $v \in \Delta_n$ is a minimizer of (SQP_{DMD}) , then $\frac{Dv}{\|Dv\|_1}$ is a minimizer of (SQP_M) . Hence, the minimizers of both problems are in one-to-one correspondence, and thus problem (SQP_M) has finitely many minimizers if and only if problem (SQP_{DMD}) has finitely many minimizers.

Now we analyze the optimality conditions (CQC), (SCC) and (SOSC) for problems (SQP_M) and (SQP_{DMD}) . Observe that the constraint qualification condition (CQC) is satisfied at every minimizer. Indeed, if $u \in \Delta_n$, then the set of inequalities that are active at u is $J(u) = \{i \in [n] : x_i = 0\} = [n] \setminus \text{Supp}(u)$, and the vectors e, e_i (for $i \in J(u)$) are linearly independent.

Let us recall a result from [4] about the support of optimal solutions for problem (SQP_M) , which we will use for the analysis of the conditions (SCC) and (SOSC). We give the short proof for clarity.

Lemma 4.5. [4, Lemma 7 (i)] *Let $M \in \text{COP}_n$ and let $x \in \mathbb{R}_+^n$ be such that $x^T Mx = 0$. Let $S = \text{Supp}(x)$ be the support of x . Then $M[S]$, the principal submatrix of M indexed by S , is positive semidefinite.*

Proof. Let $\tilde{x} = x|_S$ be the restriction of x to the coordinates indexed by S , so $\tilde{x}^T M[S]\tilde{x} = 0$. Assume by contradiction that $M[S]$ is not positive semidefinite. Then there exists $y \in \mathbb{R}^S$ such that $y^T M[S]y < 0$ and we can assume that $y^T M[S]\tilde{x} \leq 0$ (else replace y by $-y$). Since all entries of \tilde{x} are positive, there exists $\lambda \geq 0$ such that the vector $\lambda\tilde{x} + y$ has all its entries positive. Thus, $(\lambda\tilde{x} + y)^T M[S](\lambda\tilde{x} + y) = \lambda^2 \tilde{x}^T M[S]\tilde{x} + 2\lambda \tilde{x}^T M[S]y + y^T M[S]y < 0$, contradicting that $M[S]$ is copositive. \square

We now characterize the minimizers for which the strict complementarity condition (SCC) holds. Moreover, we show that, if a minimizer u of problem (SQP_M) satisfies (SCC), then the corresponding minimizer $\frac{D^{-1}u}{\|D^{-1}u\|}$ of problem (SQP_{DM}) also satisfies (SCC).

Lemma 4.6. *Let $M \in \partial\text{COP}_n$, $D \in \mathcal{D}_{++}^n$, and let u be a minimizer of problem (SQP_M) . The strict complementarity condition (SCC) holds at u if and only if $\text{Supp}(Mu) = [n] \setminus \text{Supp}(u)$ or, equivalently, $(Mu)_i > 0$ for all $i \in [n] \setminus \text{Supp}(u)$.*

As a consequence, (SCC) holds at u (for problem (SQP_M)) if and only if (SCC) holds at $\frac{D^{-1}u}{\|D^{-1}u\|}$ (for problem (SQP_{DM})).

Proof. Let $S = \text{Supp}(u)$. We first prove that $(Mu)_i = 0$ for any $i \in S$. Let $\tilde{u} = u|_S$ denote the restriction of vector u to the coordinates indexed by S . Then, we have $0 = u^T Mu = \tilde{u}^T M[S] \tilde{u}$. By Lemma 4.5, $M[S]$ is positive semidefinite, and thus $\tilde{u} \in \text{Ker}(M[S])$. Thus, $0 = (M[S] \tilde{u})_i = (Mu)_i$ for any $i \in S$. This shows $\text{Supp}(Mu) \subseteq [n] \setminus S$. Hence equality $\text{Supp}(Mu) = [n] \setminus S$ holds if and only if $(Mu)_i = \sum_{j \in \text{Supp}(u)} M_{ij} u_j > 0$ for all $i \in [n] \setminus \text{Supp}(u)$. It suffices now to show the link to (SCC).

In problem (SQP_M) the strict complementarity condition (SCC) reads:

$$Mu = \lambda e + \sum_{j \in [n] \setminus S} \mu_j e_j \quad \text{with } \mu_j > 0 \text{ for } j \in [n] \setminus S.$$

By looking at the coordinate indexed by $i \in S$ we obtain that $0 = (Mu)_i = \lambda$. Hence, $(Mu)_j = \mu_j$ for any $j \in [n] \setminus S$. Therefore (SCC) holds if and only if $(Mu)_j > 0$ for all $j \in [n] \setminus S$.

The last claim of the lemma follows using the above characterization, combined with the correspondence between the minimizers u of (SQP_M) and $D^{-1}u$ (up to scaling) of (SQP_{DM}) and the fact that $\text{Supp}(Mu) = \text{Supp}(DMu)$ and $\text{Supp}(D^{-1}u) = \text{Supp}(u)$ (as D is positive diagonal). \square

As observed, e.g., in [21], if the sufficient optimality conditions (CQC), (SCC), (SOSC) hold at every global minimizer, then the number of minimizers must be finite. We now show a useful fact: if a standard quadratic program has finitely many minimizers, then (SOSC) holds at all of them.

Lemma 4.7. *Let $M \in \partial\text{COP}_n$, so that problem (SQP_M) has optimal value zero. If (SQP_M) has finitely many minimizers, then (SOSC) holds at every global minimizer.*

Proof. Assume $M \in \partial\text{COP}_n$ and (SQP_M) has finitely many minimizers. We first prove that, given $S \subseteq [n]$, problem (SQP_M) has at most one optimal solution with support S . For this, assume by contradiction that $u \neq v \in \Delta_n$ are solutions of $x^T M x = 0$ with support S . By Lemma 4.5 the matrix $M[S]$ is positive semidefinite. Let \tilde{u} and \tilde{v} be the restrictions of the vectors u and v to the entries indexed by S . Hence, $\tilde{u}^T M[S] \tilde{u} =$

$\tilde{v}^T M[S] \tilde{v} = 0$, and thus $M[S] \tilde{u} = M[S] \tilde{v} = 0$. This implies that every convex combination of \tilde{u}, \tilde{v} belongs to the kernel of $M[S]$, so that the form $x^T M[S] x$ has infinitely many zeros on $\Delta_{|S|}$. Hence, $x^T M x$ has infinitely many zeros on Δ_n , contradicting the assumption.

Let u be a minimizer of problem (SQP_M) with support S and consider as above its restriction $\tilde{u} \in \mathbb{R}^{|S|}$. Observe that the *second order sufficiency condition* (SOSC) for problem (SQP_M) at u reads

$$v^T M v > 0 \text{ for all } v \in \mathbb{R}^n \setminus \{0\} \text{ such that } \sum_{i=1}^n v_i = 0 \text{ and } v_j = 0 \quad \forall j \in [n] \setminus S,$$

$$\text{or, equivalently, } a^T M[S] a > 0 \text{ for all } a \in \mathbb{R}^{|S|} \setminus \{0\} \text{ such that } \sum_{i \in S} a_i = 0.$$

Assume that $a^T M[S] a = 0$, we show $a = 0$. Since $M[S] \succeq 0$ we have that $M[S] a = 0$, so that $M[S](\lambda \tilde{u} + a) = 0$ for all $\lambda \in \mathbb{R}$. Pick $\lambda > 0$ large enough so that all entries of $\lambda \tilde{u} + a$ are positive. Then $\lambda \tilde{u} + a$ should be a multiple of \tilde{u} because u is the only minimizer over the simplex with support S . Combining with the fact that $e^T a = 0$ this implies $a = 0$. \square

As previously observed, the minimizers of problems (SQP_M) and (SQP_{DMD}) are in one-to-one correspondence. Thus, as a consequence of Lemma 4.7, (SOSC) holds at every global minimizer of (SQP_M) if and only if it holds at every global minimizer of problem (SQP_{DMD}) . Moreover, we have shown in Lemma 4.6 that (SCC) holds for all minimizers of problem (SQP_{DMD}) if and only if it holds for all minimizers of (SQP_M) . Therefore, we have now completed the proof of Theorem 4.4. Moreover, combining Corollary 4.3 and the characterization of (SCC) in Lemma 4.6, we obtain the following result, useful for further reference.

Theorem 4.8. *Let $M \in \partial \text{COP}_n$ and assume problem (SQP_M) has finitely many minimizers. Assume moreover that, for every minimizer u of problem (SQP_M) , we have $(Mu)_i > 0$ for all $i \in [n] \setminus \text{Supp}(u)$. Then $DMD \in \bigcup_{r \geq 0} \text{LAS}_n^{(r)}$ for all $D \in \mathcal{D}_{++}^n$.*

4.3. Proof of Theorem 2.3

Now we can prove the result of Theorem 2.3; that is, we show that $DT(\psi)D \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ for all $D \in \mathcal{D}_{++}^n$ and $\psi \in \Psi$. We show this result as a direct application of Theorem 4.8. It thus remains to check that the two assumptions in Theorem 4.8 hold. First, by combining two results from [12], the description of the (finitely many) minimizers of problem (SQP_M) for $M = T(\psi)$ ($\psi \in \Psi$) can be found.

Lemma 4.9. *The minimizers of problem (SQP_M) associated to the matrix $M = T(\psi)$ (with $\psi \in \Psi$) are the vectors $v_i = \frac{u_i}{\|u_i\|_1}$ for $i \in [5]$, where the u_i 's are defined by*

$$u_1 = \begin{pmatrix} \sin \psi_5 \\ \sin(\psi_4 + \psi_5) \\ \sin \psi_4 \\ 0 \\ 0 \end{pmatrix}, \quad u_2 = \begin{pmatrix} \sin(\psi_3 + \psi_4) \\ \sin \psi_3 \\ 0 \\ 0 \\ \sin \psi_4 \end{pmatrix}, \quad u_3 = \begin{pmatrix} 0 \\ \sin \psi_1 \\ \sin(\psi_1 + \psi_5) \\ \sin \psi_5 \\ 0 \end{pmatrix},$$

$$u_4 = \begin{pmatrix} 0 \\ 0 \\ \sin \psi_2 \\ \sin(\psi_1 + \psi_2) \\ \sin \psi_1 \end{pmatrix}, \quad u_5 = \begin{pmatrix} \sin \psi_2 \\ 0 \\ 0 \\ \sin \psi_3 \\ \sin(\psi_2 + \psi_3) \end{pmatrix}.$$

Proof. By [12, Theorem 2.5]) it follows that there are exactly five minimizers and that they are supported, respectively, by the sets $\{1, 2, 3\}$, $\{1, 2, 5\}$, $\{2, 3, 4\}$, $\{3, 4, 5\}$ and $\{1, 4, 5\}$. Next, using [12, Lemma 3.2]), we obtain that the minimizers take the desired form. \square

We finally check that the second assumption of Theorem 4.8 holds for the matrices $M = T(\psi)$ ($\psi \in \Psi$).

Lemma 4.10. *Let $\psi \in \Psi$ and let v be a minimizer of problem (SQP_M) where $M = T(\psi)$. Then, we have $(Mv)_i > 0$ for all $i \in [5] \setminus \text{Supp}(v)$.*

Proof. By symmetry, it is enough to check this condition for one of the minimizers, say v_1 (as given in Lemma 4.9). Since multiplying by a positive constant does not affect the sign we verify the condition for the vector u_1 . For convenience, we set $u = u_1$. As $\text{Supp}(u) = \{1, 2, 3\}$ the condition we want to check reads as follows

$$\sum_{i=1}^3 T(\psi)_{i4} u_i > 0 \quad \text{and} \quad \sum_{i=1}^3 T(\psi)_{i5} u_i > 0.$$

Again, it suffices to check just the first inequality since the second one is analogous (up to index permutation). We will now check that the first expression is positive. Indeed we have

$$\begin{aligned} & \sum_{i=1}^3 T(\psi)_{i4} u_i \\ &= \cos(\psi_2 + \psi_3) \sin \psi_5 + \cos(\psi_5 + \psi_1) \sin(\psi_4 + \psi_5) - \cos \psi_1 \sin \psi_4 \\ &= \cos(\psi_2 + \psi_3) \sin \psi_5 + (\cos \psi_5 \cos \psi_1 - \sin \psi_5 \sin \psi_1)(\sin \psi_4 \cos \psi_5 + \cos \psi_4 \sin \psi_5) \\ & \quad - \cos \psi_1 \sin \psi_4 \\ &= \cos(\psi_2 + \psi_3) \sin \psi_5 + (\cos^2 \psi_5 - 1) \cos \psi_1 \sin \psi_4 + \cos \psi_5 \cos \psi_1 \cos \psi_4 \sin \psi_5 \\ & \quad - \sin \psi_5 \sin \psi_1 \sin \psi_4 \cos \psi_5 - \sin^2 \psi_5 \sin \psi_1 \cos \psi_4 \\ &= \cos(\psi_2 + \psi_3) \sin(\psi_5) - \sin^2 \psi_5 \sin(\psi_1 + \psi_4) + \sin \psi_5 \cos \psi_5 \cos(\psi_1 + \psi_4) \end{aligned}$$

$$\begin{aligned}
&= \cos(\psi_2 + \psi_3) \sin \psi_5 + \sin \psi_5 \cos(\psi_1 + \psi_4 + \psi_5) \\
&= \sin \psi_5 (\cos(\psi_2 + \psi_3) + \cos(\psi_1 + \psi_4 + \psi_5)).
\end{aligned}$$

We finish the proof by showing that both factors in the last expression are positive for $\psi \in \Psi$. By the definition of Ψ , $\sum_{i=1}^5 \psi_i < \pi$ and $\psi_i > 0$ for $i \in [5]$, so that $\psi_5 \in (0, \pi)$ and thus $\sin \psi_5 > 0$. Now we use that cosine is a monotone decreasing function in the interval $(0, \pi)$. Observe that $\psi_2 + \psi_3$ and $\pi - (\psi_1 + \psi_4 + \psi_5)$ belong to $(0, \pi)$ and $\psi_2 + \psi_3 < \pi - (\psi_1 + \psi_4 + \psi_5)$. Thus, $\cos(\psi_2 + \psi_3) > \cos(\pi - (\psi_1 + \psi_4 + \psi_5)) = -\cos(\psi_1 + \psi_4 + \psi_5)$, completing the proof. \square

Remark 4.11. Our proof above for Lemma 4.10 is elementary, using only the shape of the zeros of the matrices $M = T(\psi)$ recalled in Lemma 4.9. Alternatively, as suggested by an anonymous referee, one may derive Lemma 4.10 using results from [6], as we now mention. Let v be a minimizer of problem (SQP_M) , i.e., a zero of M in Δ_n , with support $\{i, j, k\}$, and assume for contradiction that $(Mv)_\ell = 0$ for some $\ell \in [5] \setminus \{i, j, k\}$. Set $\tilde{v} := (v_i, v_j, v_k, v_\ell)$ and let $\tilde{M} \in \text{COP}_4$ be the principal submatrix of M indexed by $\{i, j, k, \ell\}$. Then we have $0 = (Mv)_h = (\tilde{M}\tilde{v})_h$ for $h \in \{i, j, k, \ell\}$, which, by [6, Corollary 4.10], implies $\tilde{M} \succeq 0$. Since, by [6, Theorem 3.1], M is irreducible with respect to the cone of nonnegative matrices, it now follows using [6, Lemma 4.12] that $M \succeq 0$, a contradiction.

5. Concluding remarks

In this paper we investigate whether the cones $\mathcal{K}_n^{(r)}$ provide a complete approximation hierarchy for the copositive cone COP_n , i.e., whether their union covers the full cone COP_n . As mentioned earlier, the answer is positive for $n \leq 4$ (then $\mathcal{K}_n^{(0)} = \text{COP}_n$ [4]) and negative for $n \geq 6$ [17]. As our main result we show that the answer is positive for $n = 5$ if and only if every positive diagonal scaling of the Horn matrix belongs to some cone $\mathcal{K}_5^{(r)}$.

Our proof technique relies on considering an alternative approximation hierarchy of COP_n , provided by the Lasserre-type cones $\text{LAS}_{\Delta_n}^{(r)} \subseteq \mathcal{K}_n^{(r)}$. Namely, we show that all the extreme matrices of COP_5 , that do not belong to $\mathcal{K}_5^{(0)}$ and are not a positive diagonal scaling of the Horn matrix, do indeed belong to $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$.

As we have seen earlier, for a matrix $M \in \text{COP}_n$, the number of zeros of the form $x^T M x$ in the simplex Δ_n plays an important role for checking membership of M in the cones $\text{LAS}_{\Delta_n}^{(r)}$. If M is strictly copositive (i.e., $x^T M x$ has no zeros in Δ_n), then $M \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$. If M has finitely many zeros in Δ_n , then, as was shown in Section 4.1, one possible strategy for showing membership in $\bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)}$ is following an optimization approach and checking the classical optimality conditions at every zero in Δ_n (i.e., every minimizer of $x^T M x$ over Δ_n). This has been our strategy for showing that every matrix $T(\psi)$ (for $\psi \in \Psi$) belongs to some cone $\text{LAS}_{\Delta_5}^{(r)}$. Finally, if $x^T M x$ has infinitely many

zeros in Δ_n , then the classical optimality conditions cannot hold and thus the strategy from Section 4.1 does not work. One example that illustrates how the number of zeros causes issues is the Horn matrix H . While H belongs to $\mathcal{K}_5^{(1)}$, it does not belong to $\text{LAS}_{\Delta_5}^{(r)}$ for any $r \in \mathbb{N}$. To show this, we have exploited the structure of the (infinitely many) zeros of the form $x^T H x$ in Δ_5 . Hence, another strategy will be needed for settling the question whether every positive diagonal scaling of H belongs to some cone $\mathcal{K}_5^{(r)}$.

In [16] we proved (rephrased in the language of the present paper) that, if G is an acritical graph, then its graph matrix M_G belongs to some cone $\text{LAS}_{\Delta_n}^{(r)}$. Our strategy there was also based on applying the optimization approach and showing that the optimality conditions hold at all the zeros of $x^T M_G x$ in Δ_n . The assumption that G is acritical indeed ensures that the number of zeros in Δ_n is finite (the zeros correspond then to the stable sets of maximum cardinality $\alpha(G)$). Therefore, as a direct application of Theorem 4.4, we obtain that every positive diagonal scaling of M_G belongs to some cone $\text{LAS}_{\Delta_n}^{(r)}$.

Corollary 5.1. *If G is an acritical graph then, for every $D \in \mathcal{D}_{++}^n$, we have $DM_G D \in \bigcup_{r \geq 0} \text{LAS}_{\Delta_n}^{(r)} \subseteq \bigcup_{r \geq 0} \mathcal{K}_n^{(r)}$.*

Dealing with general graphs (with critical edges) will likely require another strategy.

Declaration of competing interest

None declared.

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