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A variational approach to copositive matrices

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Abstract. This work surveys essential properties of the so-called copositive matrices, the study of which is spread over more than fifty-five years. Special emphasis is given to variational aspects related to the concept of copositivity. In addition, some new results on the geometry of the cone of copositive matrices are presented here for the first time.

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1 Introduction

1.1 Historical background

The concept of copositivity usually applies to a symmetric matrix or, more precisely, to its associated quadratic form. One could equally well consider a self-adjoint linear continuous operator on a Hilbert space, but in this work we stick to finite dimensionality. The definition of copositivity can be traced back to a 1952 report by Theodore S. Motzkin [85]. In the sequel, the superscript "T" indicates transposition. In particular, $x^T y = \sum_{j=1}^n x_j y_j$ corresponds to the usual inner product in the Euclidean space $\mathbb{R}^n$.

Definition 1.1. *Let A be a real symmetric matrix of order n. One says that A is copositive if its associated quadratic form $x \in \mathbb{R}^n \mapsto q_A(x) = x^T Ax$ takes only nonnegative values on the nonnegative orthant $\mathbb{R}^n_+$. Strict copositivity of A means that $x^T Ax > 0$ for all $x \in \mathbb{R}^n_+ \backslash \{0\}$.*

Of course, changing the nonnegative orthant by an arbitrary closed convex cone K would lead to a more general concept of copositivity. One could speak of copositivity relative to the ice-cream cone [41, 80], copositivity relative to a given polyhedral cone [81, 82, 100], and so on. One could even consider the case of a nonconvex cone K. The complexity of the concept of K-copositivity is very much dependent on K:

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- When $K = \{x \in \mathbb{R}^n : q_B(x) \geq 0\}$ is given by a quadratic form that is positive somewhere, the K-copositivity of A amounts to the positive semidefiniteness of $A - tB$ for some $t \in \mathbb{R}_+$; this is the so-called S- lemma of Yakubovich (*cf.* [93, 102]), an ancestor of which is the celebrated lemma of Debreu-Finsler.

- When $K = \{x \in \mathbb{R}^n : q_{B_1}(x) \geq 0, \ldots, q_{B_m}(x) \geq 0\}$ is described by means of a finite number of quadratic forms, the K-copositivity of A joins up with the notion of the *S-procedure,* which is a theory with its own motivation and field of applications (*cf.* [34, 93]).

- When $K = \mathbb{R}^n_+$, which is our case, we note immediately a conflict between the quadratic world (represented by the quadratic form q_A) and the cone K which is polyhedral. This is the main cause of all the difficulties inherent to $\mathbb{R}^n_+$- copositivity. Note incidentally that $\mathbb{R}^n_+$- copositivity and $\mathbb{R}^n_-$- copositivity amount to the same (simply because $\mathbb{R}^n_- = -\mathbb{R}^n_+$ and a quadratic form is an even function).

We do not wish to go beyond the setting of Definition 1.1, because otherwise the presentation of copositivity would be obscured by endless remarks and ramifications. As early as 1958, Gaddum [44] studied the concept of copositivity in connection with the analysis of matrix games and systems of linear inequalities. The theory of copositive matrices was consolidated in the beginning of the sixties with the pioneering contributions of Diananda [35], Hall and Newman [50], and Motzkin himself [86]. By the end of the seventies, the use of copositive matrices was already spread in many areas of applied mathematics, specially in control theory [66]. In the last decade there has been a renewal of interest in copositivity due to its impact in optimization modeling [23], linear complementarity problems [40, 69], graph theory [2, 36, 75, 92], and linear evolution variational inequalities [45].

1.2 Purpose of this work

The natural framework for discussing copositivity is the linear space $\mathbb{S}_n$ of real symmetric matrices of order n. As usual, $\mathbb{S}_n$ is equipped with the trace inner product $\langle A, B\rangle = \mathrm{tr}(AB)$ and the associated norm. The mathematical object on which our attention will be concentrated is the set

$$\mathcal{C}_n = \{A \in \mathbb{S}_n : A \text{ is copositive}\}.$$

To put everything in the right perspective, we recall at the outset of the discussion a few basic things about this set (*cf.* [49, 57] or the recent Ph.D. thesis by Bundfuss [21, Section 2.1] that we received after the first submission of this paper).

Proposition 1.2. *The set $\mathcal{C}_n$ is a closed convex cone in $\mathbb{S}_n$. Furthermore,*

(a) $\mathcal{C}_n$ has nonempty interior and is pointed in the sense that $\mathcal{C}_n \cap -\mathcal{C}_n = \{0\}$.

(b) The closed convex cones

$$\begin{aligned} \mathcal{P}_n &= \{A \in \mathbb{S}_n : A \textit{ is positive semidefinite}\}, \\ \mathcal{N}_n &= \{A \in \mathbb{S}_n : A \textit{ is nonnegative entrywise}\} \end{aligned}$$

are both contained in $\mathcal{C}_n$. Whence $\mathcal{P}_n + \mathcal{N}_n \subset \mathcal{C}_n$.

(c) $\mathcal{C}_n$ is non-polyhedral, that is to say, it cannot be expressed as the intersection of finitely many closed half-spaces.

This is more or less what every non-specialist knows about $\mathcal{C}_n$. The purpose of this work is to list the most fundamental theorems concerning the set $\mathcal{C}_n$, including negative results and open questions. We wish also to add a few contributions of our own. Linear algebraists will find of interest the good survey on copositivity written by Ikramov and Savel'eva [57], as well as the book on completely positive matrices by Berman and Shaked-Monderer [10]. In this work, special emphasis will be given to variational aspects related to the concept of copositivity. The term "variational" is not to be understood in its old historical meaning (calculus of variations), but in the broadest possible sense (optimization, game theory, complementarity problems, equilibrium problems).

Definition 1.1 is in fact related to the variational (or optimization) problem

$$\mu(A) = \min_{\substack{x \geq 0 \\ \|x\|=1}} x^T A x, \tag{1}$$

where $\|\cdot\|$ is the usual Euclidean norm and $x \geq 0$ indicates that each component of x is nonnegative. Despite its rather simple appearence, the above optimization problem offers an interesting number of challenges. Note that (1) is about minimizing a quadratic form (not necessarily convex) on a nonconvex compact portion of the nonnegative orthant.

There is yet another interesting variational problem related to copositivity. It concerns the minimization of a quadratic form on a simplex, more precisely

$$\gamma(A) = \min_{x \in \Lambda_n} x^T A x\,, \tag{2}$$

where $\Lambda_n = \{x \in \mathbb{R}^n_+ : x_1 + \ldots + x_n = 1\}$ stands for the unit-simplex of $\mathbb{R}^n$. One usually refers to (2) as the Standard Quadratic Program.

Proposition 1.3. *Let $A \in \mathbb{S}_n$. Then, the following conditions are equivalent:*

(a) A is copositive.

(b) $\mu(A)$ is nonnegative.

(c) $\gamma(A)$ is nonnegative.

The equivalence between (a) and (c) was pointed out by Micchelli and Pinkus in [83]. The full Proposition 1.3 is trivial because the cost function q_A is positively homogeneous of degree two. What is less obvious is how to compute numerically the minimal value $\mu(A)$ or the minimal value $\gamma(A)$. We shall come back to this point in Sections 4 and 5, respectively. Parenthetically, observe that the functions $\mu : \mathbb{S}_n \to \mathbb{R}$ and $\gamma : \mathbb{S}_n \to \mathbb{R}$ are positively homogeneous and concave. Hence, the representation formulas

$$\begin{aligned} \mathcal{C}_n &= \{A \in \mathbb{S}_n : \mu(A) \geq 0\} \\ &= \{A \in \mathbb{S}_n : \gamma(A) \geq 0\} \end{aligned}$$

confirm that $\mathcal{C}_n$ is a closed convex cone.

Remark 1.4. To avoid unnecessary repetitions, we rarely mention the "strict" version of copositivity. It is useful to keep in mind that

$$\begin{aligned} \{A \in \mathbb{S}_n : A \text{ is strictly copositive}\} &= \text{int}(\mathcal{C}_n), \\ \text{cl}\{A \in \mathbb{S}_n : A \text{ is strictly copositive}\} &= \mathcal{C}_n, \end{aligned}$$

where "int" and "cl" stand for topological interior and closure, respectively. In particular, a copositive matrix can be seen as a limit of a sequence of strictly copositive matrices.

2 Results valid only in small dimensions

Testing copositivity is a challenging question. For methodological reasons, we consider first the case in which the dimension n does not exceed four.

2.1 Copositivity as system of nonlinear inequalities

The two-dimensional case is clear and offers no difficulty. One simply has:

Proposition 2.1. *A symmetric matrix A of order 2 is copositive if and only if*

$$a_{1,1} \geq 0,\ a_{2,2} \geq 0, \tag{3}$$

$$a_{1,2} + \sqrt{a_{1,1}a_{2,2}} \geq 0. \tag{4}$$

As observed by Nadler [88], the system (3)-(4) is exactly what is needed for ensuring that the quadratic Bernstein-Bézier polynomial

$$p(t) = a_{1,1}(1-t)^2 + 2a_{1,2}(1-t)t + a_{2,2}t^2$$

is nonnegative on the interval $[0, 1]$. Proposition 2.1 is part of the folklore on copositive matrices and can be found in numerous references (*cf.* [1, 48, 57, 79]). By the way, the presence of the square root term in (4) confirms that $\mathcal{C}_2$ is non-polyhedral.

The three-dimensional case is still easy to handle. Checking copositivity is again a matter of testing the validity of a small system of nonlinear inequalities.

Proposition 2.2. *A symmetric matrix A of order 3 is copositive if and only if the six inequalities*

$$\begin{aligned} &a_{1,1} \geq 0,\ a_{2,2} \geq 0,\ a_{3,3} \geq 0, \\ &\bar{a}_{1,2} := a_{1,2} + \sqrt{a_{1,1}a_{2,2}} \geq 0, \\ &\bar{a}_{1,3} := a_{1,3} + \sqrt{a_{1,1}a_{3,3}} \geq 0, \\ &\bar{a}_{2,3} := a_{2,3} + \sqrt{a_{2,2}a_{3,3}} \geq 0, \end{aligned}$$

are satisfied, as well as the last condition

$$\sqrt{a_{1,1}a_{2,2}a_{3,3}} + a_{1,2}\sqrt{a_{3,3}} + a_{1,3}\sqrt{a_{2,2}} + a_{2,3}\sqrt{a_{1,1}} + \sqrt{2\,\bar{a}_{1,2}\,\bar{a}_{1,3}\,\bar{a}_{2,3}} \geq 0. \tag{5}$$

The above proposition can be found, for instance, in Chang and Sederberg [25]. There are seven inequalities in all, the last one being the only one that looks a bit bizarre. The first six inequalities simply say that the principal submatrices

$$\begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{1,2} & a_{2,2} \end{bmatrix}, \begin{bmatrix} a_{1,1} & a_{1,3} \\ a_{1,3} & a_{3,3} \end{bmatrix}, \begin{bmatrix} a_{2,2} & a_{2,3} \\ a_{2,3} & a_{3,3} \end{bmatrix}$$

of order 2 are copositive. A variant of Proposition 2.2 was suggested earlier by Hadeler [48, Theorem 4]. It consists in writing the inequality (5) in the disjunctive form

$$\det A \geq 0 \quad \text{or} \quad \sqrt{a_{1,1}a_{2,2}a_{3,3}} + a_{1,2}\sqrt{a_{3,3}} + a_{1,3}\sqrt{a_{2,2}} + a_{2,3}\sqrt{a_{1,1}} \geq 0.$$

There is also a "strict" version of Proposition 2.2 due to Simpson and Spector [99, Theorem 2.2]. The latter authors applied such a proposition for characterizing strong ellipticity in isotropic elastic materials. In connection with this theme, see also the work by Kwon [77].

Remark 2.3. The case $n = 4$ is treated by Li and Feng [79]. Their results are displayed by case analysis. According to the sign distribution of the off-diagonal entries of A, eight different subcases are to be considered. Writing down all the details is space consuming and, besides, it does not provide a good insight on what could happen in higher dimensions.

2.2 Diananda's decomposition

As observed in Proposition 1.2, one has $\mathcal{P}_n + \mathcal{N}_n \subset \mathcal{C}_n$ for any dimension n. In a celebrated paper of 1962, Diananda [35] observed that the reverse inclusion is true if n does not exceed four.

Theorem 2.4. *Let $n \leq 4$. Then, $\mathcal{C}_n = \mathcal{P}_n + \mathcal{N}_n$.*

In words, a symmetric matrix A of order $n \leq 4$ is copositive if and only if it is decomposable as sum $A = A_1 + A_2$ of a positive semidefinite symmetric matrix A_1 and a nonnegative symmetric matrix A_2. Curiously enough, Diananda's decomposition theorem fails for $n \geq 5$. This can be seen by working out the counter-example

$$A = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}$$

proposed by A. Horn (*cf.* [35]). The above matrix is copositive, but it cannot be decomposed in the requested form. We mention in passing a beautiful paper by Cottle [27] with a long list of theorems that are valid up to $n = 4$, but not beyond this threshold.

Remark 2.5. The set $\mathcal{P}_n + \mathcal{N}_n$ is a closed convex cone. A matrix $A \in \mathcal{C}_n$ which is not in $\mathcal{P}_n + \mathcal{N}_n$ is said to be "exceptional". A general mechanism for constructing exceptional matrices is proposed in [68].

3 Recursive strategies for detecting copositivity

There is an obvious link between the copositivity of a matrix of order n and the copositivity of its principal submatrices of order $n-1$. If one sets a particular component of $x \in \mathbb{R}^n$ equal to zero, then $q_A(x)$ becomes a quadratic form in the remaining variables. One thus clearly has:

Proposition 3.1. *If $A \in \mathcal{S}_n$ is copositive, then each principal submatrix of A of order $n-1$ is copositive.*

Of course, one can apply Proposition 3.1 recursively. If $A \in \mathcal{S}_n$ is copositive, then a principal submatrix of any order less than n is also copositive. Writing the converse of Proposition 3.1 is a more delicate matter. Suppose that A is a symmetric matrix of order n such that each principal submatrix of order $n-1$ is copositive. What exactly must be added to make sure that A itself is copositive?

3.1 Gaddum's copositivity test

Gaddum [44, Theorem 3.2] answers the above question by using the formalism of two-person zero-sum matrix games.

Theorem 3.2. *Let A be a symmetric matrix of order n such that each principal submatrix of order $n-1$ is copositive. Then, A is copositive if and only if the value*

$$\mathrm{val}(A) := \min_{x \in \Lambda_n} \max_{y \in \Lambda_n} y^T A x = \max_{y \in \Lambda_n} \min_{x \in \Lambda_n} y^T A x \tag{6}$$

of the matrix game induced by A is nonnegative.

The second equality in (6) is just a reminder of von Neumann's minimax theorem. The important point concerning the formulation of Theorem 3.2 is that $\mathrm{val}(A)$ can be computed by solving a standard linear programming problem, namely

$$\begin{array}{l} \text{minimize} \quad t_1 - t_2 \\ x_1 + \ldots + x_n = 1 \\ a_i^T x - t_1 + t_2 + s_i = 0 \quad i = 1, \ldots n \\ (x, s, t) \in \mathbb{R}^{2n+2}_+ \end{array}$$

with a_i standing for the i-th column of A.

Gaddum's copositivity test is of interest only if the dimension n is moderate. If $f_{\mathrm{game}}(k)$ represents the cost of evaluating the value of a matrix game of order k, then the cost of checking the copositivity of a matrix of order n is given by

$$F_{\mathrm{game}}(n) = \sum_{k=1}^{n} C_n^k \, f_{\mathrm{game}}(k)$$

with $C_n^k = n!/\left[k!(n-k)!\right]$ standing for the usual binomial coefficient. In practice, the implementation of Gaddum's copositivity test is a reasonable option when n does not exceed twenty. Of course, the final word is given by the quality of the matrix game solver.

3.2 The copositivity test of Cottle-Habetler-Lemke

The approach of Cottle, Habetler, and Lemke [28, 29] differs substantially from Gaddum's one. Instead of computing values of matrix games, the main task now consists in computing determinants and adjugate matrices.

Theorem 3.3. *Let A be a symmetric matrix of order n such that each principal submatrix of order $n-1$ is copositive. Then,*

$$A \text{ is copositive} \iff \det A \geq 0 \text{ or } \operatorname{adj} A \text{ contains a negative entry.} \tag{7}$$

Adjugation of a square matrix is defined as usual, *i.e.*, the adjugate matrix $\operatorname{adj} A$ is the transpose of the matrix of cofactors of A (*cf.* [55]). Given that A is assumed to be symmetric, transposition is unnecessary after forming the matrix of cofactors. The equivalence (7) is sometimes rephrased in a negative form. In such a way, one sees that checking copositivity boils down to inverting a family of $2^n - 1$ matrices of different sizes.

Theorem 3.4. *Let A be a symmetric matrix of order n such that each principal submatrix of order $n-1$ is copositive. Then,*

$$A \text{ is not copositive} \iff A^{-1} \text{ exists and is nonpositive entrywise.}$$

A short proof of Theorem 3.4 can be found in Hadeler [48]. These results pertain to the realm of classical matrix analysis, so we shall not insist too much on them. Additional comments on copositivity and invertibility will be given in Section 7.4.

3.3 A copositivity test for specially structured matrices

The next theorem can be traced back to Bomze [11, 12], see also [1, 67, 79]. Other results in the same spirit, but involving more general Schur complements, are proposed in [14, Theorem 5] and [17, Theorem 2].

Theorem 3.5. *Let $b \in \mathbb{R}^{n-1}$ and $C \in \mathbb{S}_{n-1}$. The matrix*

$$A = \begin{bmatrix} a & b^T \\ b & C \end{bmatrix} \in \mathbb{S}_n \tag{8}$$

is copositive if and only if the following conditions are satisfied:

i) $a \geq 0$, C is copositive,

ii) $y^T(aC - bb^T)y \geq 0$ for all $y \in \mathbb{R}^{n-1}_+$ such that $b^T y \leq 0$.

The most bothersome aspect of Theorem 3.5 is the verification of (ii). What this condition says is that $aC - bb^T \in \mathbb{S}_{n-1}$ is copositive relative to the closed convex cone

$$\{y \in \mathbb{R}^{n-1} : y \geq 0, b^T y \leq 0\}.$$

There is an alternative formulation of (ii) that deserves a special mention. If one enters into the proof of [79, Theorem 2], then one realizes that the matrix in (8) is copositive if and only if

$$\begin{bmatrix} a & b^T y \\ b^T y & y^T C y \end{bmatrix} \in \mathcal{C}_2 \qquad \text{for all } y \in \mathbb{R}^{n-1}_+. \tag{9}$$

In other words, everything boils down to checking copositivity of a symmetric matrix of order 2. If one applies Proposition 2.1 to the matrix appearing in (9), then one obtains (i) and the extra condition

$$b^T y + \sqrt{a}\sqrt{y^T C y} \geq 0 \qquad \text{for all } y \in \mathbb{R}^{n-1}_+. \tag{10}$$

The inequality (10) is undoubtedly a simpler way of formulating (ii). By a positive homogeneity argument, the condition (ii) then amounts to saying that the minimal value

$$\min_{y \in \Lambda_{n-1}} \left\{ b^T y + \sqrt{a}\sqrt{y^T C y} \right\} \tag{11}$$

is nonnegative. Although the above variational problem does not look easier than (2), one must observe that the minimization vector in (11) ranges over a simplex of smaller dimension.

Remark 3.6. When $n = 3$, the variational problem (11) consists simply in minimizing

$$g(t) = a_{1,2}t + a_{1,3}(1-t) + \sqrt{a_{1,1}}\,\sqrt{a_{2,2}t^2 + 2a_{2,3}\,t(1-t) + a_{3,3}(1-t)^2}$$

over the interval $[0, 1]$. This leads to the bizarre inequality (5) of Proposition 2.2.

We end this section with two immediate by-products of Theorem 3.5. The first corollary appears in [79, Theorem 3], while the second one is a result proposed in [87, Exercise 3.53].

Corollary 3.7. *Suppose that b is a nonpositive vector in $\mathbb{R}^{n-1}$ and that $C \in \mathbb{S}_{n-1}$. Then,*

$$\begin{bmatrix} a & b^T \\ b & C \end{bmatrix} \text{ is copositive} \quad \Longleftrightarrow \quad a \geq 0 \text{ and } C,\ aC - bb^T \text{ are copositive}$$

$$\Longleftrightarrow \quad \begin{cases} \text{either } a = 0,\ b = 0 \text{ and } C \text{ is copositive} \\ \text{or } a > 0 \text{ and } aC - bb^T \text{ is copositive.} \end{cases}$$

Corollary 3.8. *Suppose that the off-diagonal entries of $A \in \mathbb{S}_n$ are all nonpositive. Then, A is copositive if and only if A is positive semidefinite.*

4 Results involving classical eigenvalues and Pareto eigenvalues

4.1 Spectral properties of copositive matrices

Even if all the eigenvalues of $A \in \mathbb{S}_n$ are known, this information alone is not enough to decide whether A is copositive or not.

Proposition 4.1. *Let $A \in \mathbb{S}_n$.*

(a) If A is copositive, then at least one of the eigenvalues of A is nonnegative (in fact, the sum of all the eigenvalues of A, counting multiplicity, is nonnegative).

(b) If all the eigenvalues of A are nonnegative, then A is copositive (in fact, positive semidefinite).

For proving (a) note that the diagonal entries of a copositive matrix are nonnegative and its trace is equal to the sum of the eigenvalues. Needless to say, Proposition 4.1 is very crude. What is important to know about $A \in \mathbb{S}_n$ is not its usual spectrum, but its so-called Pareto spectrum. The concept of Pareto eigenvalue is not associated with the classical Rayleigh-Ritz minimization problem

$$\lambda_{\min}(A) = \min_{\|x\|=1} x^T A x \,,$$

but with the cone-constrained minimization problem (1). The minimal value $\mu(A)$ defined in (1) is a mathematical expression of interest by its own sake. Such a term appears once and over again in diverse situations (*cf.* [46, 47]). By writing down the optimality conditions for problem (1), one arrives at a complementarity system of the form

$$x \geq 0, \quad Ax - \lambda x \geq 0, \quad x^T(Ax - \lambda x) = 0, \tag{12}$$

$$\|x\| = 1, \tag{13}$$

where $\lambda \in \mathbb{R}$ is viewed as a Lagrange multiplier associated with the normalization constraint (13). The definition below is taken from Seeger [96]. It applies to an arbitrary matrix, be it symmetric or not.

Definition 4.2. *Let A be a real matrix of order n. The number $\lambda \in \mathbb{R}$ is called a Pareto eigenvalue of A if the complementarity system (12) admits a nonzero solution $x \in \mathbb{R}^n$. The set of all Pareto eigenvalues of A, denoted by $\Pi(A)$, is called the Pareto spectrum of A.*

Theoretical results and algorithms for computing Pareto spectra can be found in [96, 97, 98] and [70, 71, 90, 91, 94], respectively. The next theorem displays the link between Pareto spectra and copositivity.

Theorem 4.3. *A symmetric matrix A of order n is copositive if and only if all the Pareto eigenvalues of A are nonnegative.*

The proof of Theorem 4.3 is not too difficult. The key observation is that, in the symmetric case, the coefficient $\mu(A)$ turns out to be the smallest element of $\Pi(A)$. In short,

$$\mu(A) = \min_{\lambda \in \Pi(A)} \lambda.$$

The proposition below, taken from [96], tells us how to compute Pareto spectra in practice. In what follows, $\mathcal{J}(n)$ denotes the collection of all nonempty subsets of $\{1, \ldots, n\}$, the symbol $|J|$ stands for the cardinality of $J \in \mathcal{J}(n)$, and A^J refers to the principal submatrix of A formed with the rows and columns of A indexed by J.

Proposition 4.4. *Let A be a matrix of order n. Then, $\lambda \in \Pi(A)$ if and only if there are an index set $J \in \mathcal{J}(n)$ and a vector $\xi \in \mathbb{R}^{|J|}$ such that*

$$A^J \xi = \lambda \xi \tag{14}$$

$$\xi \in \mathrm{int}(\mathbb{R}^{|J|}_+) \tag{15}$$

$$\sum_{j \in J} A_{ij} \xi_j \geq 0 \quad \forall i \notin J. \tag{16}$$

Computing a Pareto spectrum is a much harder problem than computing a usual spectrum. In the first case one has to take into consideration all the possible ways of selecting the index set J. In practice, one has to solve $2^n - 1$ classical eigenvalue problems. To be more precise, one has to solve (14)-(16) for each principal submatrix of A. Keeping in mind Proposition 4.4, one can see the next result by Kaplan [73, 74] as a simplification of Theorem 4.3. What Kaplan suggests, in fact, is testing copositivity by working out (14)-(15) and neglecting (16).

Corollary 4.5. *A symmetric matrix A of order n is copositive if and only if*

$$A^J\xi = \lambda\xi \quad \textit{and} \quad \xi \in \operatorname{int}(\mathbb{R}^{|J|}_+) \quad \Longrightarrow \quad \lambda \geq 0$$

for every nonempty index set $J \subset \{1, \ldots, n\}$.

Kaplan's corollary is perhaps better understood if one introduces the concept of interior eigenvalue.

Definition 4.6. *Let A be a real matrix of order n. A real eigenvalue of A associated with an eigenvector with positive components is called an interior eigenvalue of A. The set of all interior eigenvalues of A is denoted by $\sigma_{\text{int}}(A)$.*

As shown by Seeger and Torki [98], for a symmetric matrix A, one always has

$$\mu(A) = \min_{J \in \mathcal{J}(n)} \inf_{\lambda \in \sigma_{\text{int}}(A^J)} \lambda\,, \tag{17}$$

where the inner infimum is defined as $+\infty$ if the principal submatrix A^J does not admit interior eigenvalues. This explains why the condition (16) is irrelevant when it comes to check copositivity.

If $f_{\text{spec}}(k)$ represents the cost of computing the eigenvalues of a matrix of order k, then the cost of checking the copositivity of a matrix of order n is given by

$$F_{\text{spec}}(n) = \sum_{k=1}^{n} C_n^k\, f_{\text{spec}}(k).$$

As was the case with Gaddum's method, the implementation of Kaplan's copositivity test is a viable option only if the dimension n is moderate. According to our computational experience, Kaplan's method must be abandoned when n is larger than 20.

4.2 Dual interpretation of the smallest Pareto eigenvalue

The minimal value of the variational problem (1) admits the inf-sup formulation

$$\mu(A) = \inf_{x \geq 0} \sup_{\lambda \in \mathbb{R}} L(x, \lambda)$$

with $L(x, \lambda) = x^T Ax - \lambda(x^T x - 1)$. By exchanging the order of the infimum and the supremum one gets

$$\beta(A) = \sup_{\lambda \in \mathbb{R}} \inf_{x \geq 0} L(x, \lambda),$$

which, after a short simplification, yields

$$\beta(A) = \sup\{\lambda \in \mathbb{R} : A - \lambda I_n \in \mathcal{C}_n\} \tag{18}$$

with I_n denoting the identity matrix of order n. One refers to (18) as the dual problem associated with (1). Although the Lagrangean function $L : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ is not convex with respect to the minimization vector x, there is no duality gap between the primal problem (1) and its dual (18). The proposition below is a particular case of a more general result taken from [98].

Proposition 4.7. *Let $A \in \mathbb{S}_n$. Then,*

(a) There is no duality gap between (1) and (18), i.e., $\mu(A) = \beta(A)$.

(b) The dual problem (18) has exactly one global solution, namely $\lambda = \mu(A)$.

A key observation concerning the minimization problem (1) is that the cost function q_A is positively homogeneous (of degree 2) and the constraint function $\|\cdot\|$ is nonnegative and positively homogeneous (of degree 1). Proposition 4.7 can be obtained from a general duality result on minimization problems with positively homogeneous data.

5 Copositivity and the Standard Quadratic Program

This section discusses copositivity in connection with the Standard Quadratic Program (2). As shown in the review paper by Bomze [16], the Standard Quadratic Program arises in many areas, including graph theory, portfolio optimization, game theory, and population dynamics.

5.1 Dual interpretation of $\gamma(A)$

Sometimes one writes the Standard Quadratic Program in the equivalent form

$$\gamma(A) \quad = \quad \min\{x^T A x : x \geq 0,\ x^T \mathbf{1_n} \mathbf{1_n}^T x = 1\}$$

with $\mathbf{1}_n = (1, \ldots, 1)^T \in \mathbb{R}^n$ denoting a vector of ones. Of course, $\mathbf{1_n} \mathbf{1_n}^T$ is the matrix of order n with ones everywhere. If one exchanges the order of the infimum and the supremum in the inf-sup formulation

$$\gamma(A) = \inf_{x \geq 0} \sup_{\lambda \in \mathbb{R}} \left\{ x^T A x - \lambda (x^T \mathbf{1_n} \mathbf{1_n}^T x - 1) \right\},$$

then one ends up with the dual problem

$$\delta(A) = \sup\{\lambda \in \mathbb{R} : A - \lambda\, \mathbf{1_n} \mathbf{1_n}^T \in \mathcal{C}_n\}. \tag{19}$$

Similarly as in Section 4.2, one gets:

Proposition 5.1. *Let $A \in \mathbb{S}_n$. Then,*

(a) There is no duality gap between (2) and (19), i.e., $\gamma(A) = \delta(A)$.

(b) The dual problem (19) has exactly one global solution, namely $\lambda = \gamma(A)$.

The equality between $\gamma(A)$ and $\delta(A)$ has been pointed out by de Klerk and Pasechnik (*cf.* [75, 76]). Such an equality corresponds to a particular instance of a general duality result from the theory of linear conic programming.

5.2 LP reformulation of $\gamma(A)$

As shown by de Klerk and Pasechnik [76], the minimization problem (2) can be converted into a linear program. The price to pay for this simplification is the introduction of a huge number of optimization variables. The mechanism that transforms (2) into a linear program is explained next. The basic idea is exploiting the theorem stated below, which is yet another contribution of Gaddum [44] to the theory of copositive matrices.

Theorem 5.2. *For $A \in \mathbb{S}_n$, the following statements are equivalent:*

i) A is copositive,

ii) For all $J \in \mathcal{J}(n)$, the system $A^J\xi \geq 0$ admits a nonzero solution $\xi \in \mathbb{R}_+^{|J|}$.

By homogeneity, there is no loss of generality in asking the entries of ξ to sum up to one. A nice and short proof of Theorem 5.2 can be found in [76]. If one applies Theorem 5.2 for characterizing the copositivity constraint $A - \lambda \mathbf{1_n}\mathbf{1_n}^T \in \mathcal{C}_n$ in problem (19), then, after a short simplification, one ends up with the linear program

$$\gamma(A) = \max\left\{\lambda : A^J x_J - \lambda \mathbf{1}_{|J|} \geq 0,\, x_J \geq 0,\, \mathbf{1}_{|J|}^T x_J = 1 \text{ for all } J \in \mathcal{J}(n)\right\}. \tag{20}$$

Of course, $\mathbf{1}_{|J|}$ is a vector of ones, the subscript being used for indicating its dimension. The maximization variables in (20) are λ and the components of the different vectors x_J's. There are

$$1 + \sum_{k=1}^{n} k\, C_n^k = 1 + \frac{1}{2} n 2^n$$

maximization variables in all, a number that grows exponentially with the dimension n. An exponential growth is also observed when its comes to count the number of constraints in (20). There are $2^n - 1$ equality constraints plus $n2^n$ inequality constraints (including the nonnegativity of the variables).

5.3 Quartic reformulation of $\gamma(A)$

As explained by Bomze and Palagi [20], it is possible to get rid of the nonnegativity constraints $x_j \geq 0$ in (2) by writing $x_j = u_j^2$. The condition $\mathbf{1_n}^T x = 1$ becomes $\|u\|^2 = 1$, and one finally gets at the ball-constrained minimization problem

$$\gamma(A) = \min_{\|u\|^2=1} \sum_{i,j=1}^{n} a_{i,j} u_i^2 u_j^2. \tag{21}$$

A careful analysis of problem (21) is carried out in [20]. Although the feasible set in (21) is quite simple, one should not be overly optimistic about this reformulation of $\gamma(A)$. Anyway, what is important to retain is the following corollary.

Corollary 5.3. *$A \in \mathbb{S}_n$ is copositive if and only if the quartic multivariate polynomial*

$$u \in \mathbb{R}^n \mapsto p_A(u) = \sum_{i,j=1}^{n} a_{i,j} u_i^2 u_j^2$$

is nonnegative everywhere (or, equivalently, nonnegative on the unit vector sphere of $\mathbb{R}^n$).

With Corollary 5.3 one enters the classical domain of mathematics dealing with the nonnegativity of multivariate polynomials. We shall come back to this theme in Section 8.1.

5.4 Comparison between $\gamma(A)$ and $\mu(A)$

Is there any order relationship between the functions $\gamma : \mathbb{S}_n \to \mathbb{R}$ and $\mu : \mathbb{S}_n \to \mathbb{R}$? The following example shows that neither one of these functions is pointwisely greater than the other.

Example 5.4. Consider the matrices

$$A = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}, \quad A' = \begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix}.$$

On the one hand, $\mu(A) = 2$ is bigger than $\gamma(A) = 1$, but, on the other hand, $\mu(A') = -2$ is smaller than $\gamma(A') = -1$. So, the functions γ and μ simply cannot be compared.

Both γ and μ can be immersed in a special class $\{F_p\}_{p\geq 1}$ of functions $F_p : \mathbb{S}_n \to \mathbb{R}$ of the type

$$F_p(A) = \min_{B\in\Delta_p} \langle B, A\rangle,$$

i.e., representable as lower envelope of linear forms. The supporting set Δ_p is here a compact convex set of $\mathbb{S}_n$, namely

$$\Delta_p = \mathrm{co}\{xx^T : x \geq 0,\, x_1^p + \ldots + x_n^p = 1\}.$$

As usual, "co" indicates the convex hull operation.

Proposition 5.5. *For all $p, q \geq 1$, one has*

$$\sup_{\|A\|=1} |F_p(A) - F_q(A)| = \mathrm{haus}(\Delta_p, \Delta_q), \tag{22}$$

where "haus" stands for the Pompeiu-Hausdorff metric on the nonempty compact subsets of $\mathbb{S}_n$. In particular,

$$|\gamma(A) - \mu(A)| \leq \mathrm{haus}(\Delta_1, \Delta_2)\|A\| \quad \textit{for all } A \in \mathbb{S}_n. \tag{23}$$

Formula (22) follows from the well known support function characterization of the Pompeiu-Hausdorff metric. The concept of support function is standard in convex analysis [53], so we can dispense with its formal presentation. What we wish to retain from Proposition 5.5 is the inequality (23). The term $\mathrm{haus}(\Delta_1, \Delta_2)$ is the smallest constant that one can put in front of $\|A\|$. Although γ and μ are not comparable in the pointwise ordering sense, these functions are somewhat related after all.

Remark 5.6. We mention in passing that (1) and (2) are particular instances of the variational problem

$$\text{minimize} \quad \left\{ \sum_\alpha c_\alpha x_1^{\alpha_1} \cdots x_n^{\alpha_n} \,:\, x \geq 0, x_1^p + \ldots + x_n^p = 1 \right\}, \tag{24}$$

where the summation index $\alpha = (\alpha_1, \ldots, \alpha_n)$ ranges over a finite set and the c_α's are given coefficients. As explained in [4], such a minimization problem arises in pattern recognition, image processing, and other areas of applied mathematics. The reader interested in the analysis of (24) may consult [4] and references therein. See also [78] for related material.

6 The convex cone $\mathcal{C}_n$ of copositive matrices

6.1 Dual cone of $\mathcal{C}_n$

Copositivity is a rather mild form of positivity. There exists another concept of positivity which is much stronger. It reads as follows:

Definition 6.1. *A symmetric matrix B of order n is completely positive if one can find an integer m and a matrix F of size $n \times m$ with nonnegative entries such that $B = FF^T$. The smallest possible number m is called the CP-rank of B.*

The above concept of positivity goes back to Hall and Newman [50] at least. According to Berman and Plemmons [9], the first application of this concept was block designs in Hall [49]. The recent book by Berman and Shaked-Monderer [10] is devoted to the study of completely positive matrices, but the emphasis there is not on variational aspects.

It is fairly easy to prove that the set

$$\mathcal{G}_n = \{B \in \mathbb{S}_n : B \text{ is completely positive}\}$$

is a closed convex cone in $\mathbb{S}_n$. Furthermore, $\mathcal{G}_n$ has nonempty interior and is pointed. In fact, all these observations follow from the next duality result already established by Hall [49].

Theorem 6.2. *$\mathcal{C}_n$ and $\mathcal{G}_n$ are dual to each other in the sense that*

$$\begin{aligned} \mathcal{G}_n &= \{B \in \mathbb{S}_n : \langle A, B\rangle \geq 0 \text{ for all } A \in \mathcal{C}_n\}, \\ \mathcal{C}_n &= \{A \in \mathbb{S}_n : \langle A, B\rangle \geq 0 \text{ for all } B \in \mathcal{G}_n\}. \end{aligned}$$

The convex cone $\mathcal{N}_n$ is self-dual, and so is the convex cone $\mathcal{P}_n$. Hence, Diananda's decomposition theorem can be reformulated as follows.

Corollary 6.3. *Let $n \leq 4$. Then, $\mathcal{G}_n = \mathcal{P}_n \cap \mathcal{N}_n$.*

Regardless of the dimension n, one always has the inclusion $\mathcal{G}_n \subset \mathcal{P}_n \cap \mathcal{N}_n$. By the way, the matrices in $\mathcal{P}_n \cap \mathcal{N}_n$ sometimes are called "doubly nonnegative". Of course, in dimension $n \geq 5$ there are matrices which are doubly nonnegative but not completely positive. The counter-example

$$A = \begin{bmatrix} 4 & 0 & 0 & 2 & 2 \\ 0 & 4 & 3 & 0 & 2 \\ 0 & 3 & 4 & 2 & 0 \\ 2 & 0 & 2 & 4 & 0 \\ 2 & 2 & 0 & 0 & 4 \end{bmatrix}$$

proposed by Hall [49] illustrates this point; see also [24].

We comment in passing that the problem of characterizing the interior of $\mathcal{G}_n$ is treated in [37]. Also, there is a vast literature devoted to the problem of estimating the CP-rank of a completely copositive matrix. This topic falls beyond the context of our survey, but the reader may find relevant information in the books [9, 10] and references therein.

6.2 Boundary of $\mathcal{C}_n$

Is it easy to recognize the boundary points of $\mathcal{C}_n$? The answer is yes if one admits that the evaluation of $\mu : \mathbb{S}_n \to \mathbb{R}$ can be carried out without trouble. Indeed, the boundary of $\mathcal{C}_n$ is representable in the form

$$\partial\mathcal{C}_n = \{A \in \mathbb{S}_n : \mu(A) = 0\}. \tag{25}$$

In other words, $A \in \mathbb{S}_n$ is a boundary point of $\mathcal{C}_n$ if and only if the smallest Pareto eigenvalue of A is equal to 0. One must keep in mind, however, that Pareto spectra are difficult to compute when the dimension n is larger than 20. Of course, if one considers the alternative characterization

$$\partial\mathcal{C}_n = \{A \in \mathbb{S}_n : \gamma(A) = 0\},$$

then everything boils down to evaluating $\gamma : \mathbb{S}_n \to \mathbb{R}$ in an efficient manner. Anyway, by combining (25) and (17), one gets the following by-product.

Corollary 6.4. *Let $A \in \mathbb{S}_n$ be copositive. Then, A belongs to $\partial\mathcal{C}_n$ if and only if $A^J\xi = 0$ for some index set $J \in \mathcal{J}(n)$ and some vector $\xi \in \mathbb{R}^{|J|}$ with positive components.*

Remark 6.5. As a direct by-product of Corollary 6.4, one has the following necessary condition for membership in $\partial\mathcal{C}_n$: every matrix in $\partial\mathcal{C}_n$ admits a principal submatrix whose determinant is equal to zero.

6.3 Extreme rays and faces of $\mathcal{C}_n$

The question of characterizing the extreme rays of $\mathcal{C}_n$ was addressed already in the sixties by Hall and Newman [50], Baumert [7, 8], and Baston [6]. The classical definition of extreme ray adjusted to the case of the cone $\mathcal{C}_n$ reads as follows:

Definition 6.6. *An extreme ray of $\mathcal{C}_n$ is a set of the form $\mathbb{R}_+A$, where $A \in \mathbb{S}_n$ is a nonzero copositive matrix such that*

$$A = A_1 + A_2 \ (\textit{with } A_1, A_2 \in \mathcal{C}_n) \quad \Longrightarrow \quad \begin{cases} \textit{there exists } t \in [0,1] \textit{ such that} \\ A_1 = (1-t)A \textit{ and } A_2 = tA. \end{cases}$$

By abuse of language, a matrix A as in Definition 6.6 is called an *extreme copositive matrix*. The term "extreme copositive" is also used while referring to the associated quadratic form. The theory of extreme copositive matrices is highly technical and it would be too space consuming entering into the details. Nonetheless, mentioning a few simple results could be a welcome introduction to the topic.

Clearly, any extreme copositive matrix of order n belongs to $\partial\mathcal{C}_n$. However, a nonzero matrix in $\partial\mathcal{C}_n$ does not need to be an extreme copositive matrix. For instance, the matrix

$$\begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{26}$$

is in the boundary of $\mathcal{C}_2$, but it is not extreme. Below we state a theorem by Hall and Newman [50] which takes place in dimension $n \in \{2, 3, 4\}$. Recall that in such low dimensions one can rely on Diananda's decomposition theorem.

Theorem 6.7. *Let $n \in \{2,3,4\}$. The extreme copositive quadratic forms in n variables are of three types:*

i) ax_k^2, *where* $a > 0$ *and* $k \in \{1,\dots,n\}$.

ii) bx_kx_ℓ, *where* $b > 0$ *and* $k,\ell \in \{1,\dots,n\}, k \neq \ell$.

iii) $\left(\sum_{i\in I} a_ix_i - \sum_{j\in J} b_jx_j\right)^2$, *where each* a_i *is positive, each* b_j *is positive, and the nonempty index sets* $I, J \subset \{1,\dots,n\}$ *are disjoint.*

For instance, the extreme copositive matrices of order two are

$$\underbrace{\begin{bmatrix} a & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & b \end{bmatrix}}_{type\,(i)}, \quad \underbrace{\begin{bmatrix} 0 & b \\ b & 0 \end{bmatrix}}_{type\,(ii)}, \quad \underbrace{\begin{bmatrix} a^2 & -ab \\ -ab & b^2 \end{bmatrix}}_{type\,(iii)}$$

with $a > 0$ and $b > 0$. In dimension $n = 3$, an example of an extreme copositive matrix of type (iii) is

$$\begin{bmatrix} a_1^2 & a_1a_2 & -a_1b_3 \\ a_1a_2 & a_2^2 & -a_2b_3 \\ -a_1b_3 & -a_2b_3 & b_3^2 \end{bmatrix}$$

with $a_1, a_2, b_3 > 0$. This corresponds to the particular choice $I = \{1,2\}$ and $J = \{3\}$.

For $n \geq 5$, the extreme rays of $\mathcal{C}_n$ include the three types mentioned in Theorem 6.7, but there are other more involved types as well. The next theorem by Baumert [7] provides a necessary condition for extreme copositivity. This time, no restriction on the dimension n is imposed. Of course, the case $n = 1$ is automatically ruled out because it has no interest.

Theorem 6.8. *Let $A \in \mathbb{S}_n$ be an extreme copositive matrix. Then, for all indices $k \in \{1,\dots,n\}$, the following equivalent conditions hold:*

(a) $u^TAu = 0$ *for some* $u \in \Lambda_n$ *such that* $u_k > 0$.

(b) For any $\varepsilon > 0$, *the shifted quadratic form* $x \in \mathbb{R}^n \mapsto x^TAx - \varepsilon x_k^2$ *is not copositive.*

Baumert's theorem is quite elegant, but it does not fully answer the question of characterizing extreme copositivity. To the best of our knowledge, a complete and tractable characterization of extreme copositivity for $n \geq 5$ has not been given so far.

Under additional structural assumptions on $A \in \mathbb{S}_n$ (for instance, specific constraints affecting one or more entries of the matrix), it is possible to decide whether $A \in \mathbb{S}_n$ is extreme copositive or not. In this category of works, one can mention the contributions of Baston [6], Hoffman and Pereira [54], Haynsworth and Hoffman [52], and others. But, as said before, the general case is still waiting for a satisfactory answer.

The theory of faces of convex cones (*cf.* [5]) goes far beyond the concept of extreme ray. In the parlance of facial analysis, extreme rays correspond to one dimensional faces. The boundary of any closed convex cone can be partioned into its faces. Some faces are one dimensional, some others are two dimensional, and so on. In general, not all the dimensions show up in the facial partition of the boundary. For instance, the ice-cream cone in $\mathbb{R}^3$ does not admit two dimensional faces.

Identifying the higher dimensional faces of $\mathcal{C}_n$ is even more complicated than finding its extreme rays. The following proposition is elementary and does not reflect the complexity of the facial detection problem. We mention this proposition because we want to emphasize that some portions of $\partial\mathcal{C}_n$ exhibit a sort of curvature like in a revolution cone, but other portions are flat like in a polyhedral cone.

Proposition 6.9. *For all $n \geq 2$, there are linearly independent matrices $A_1, A_2 \in \mathbb{S}_n$ such that*

$$\text{cone}\{A_1, A_2\} = \{t_1 A_1 + t_2 A_2 : t_1, t_2 \geq 0\} \tag{27}$$

is contained in $\partial\mathcal{C}_n$. One can choose A_1, A_2 as being extreme copositive, so that (27) is a two dimensional face of $\mathcal{C}_n$.

Proof. Let $n = 2$. Inspired by (26) and Theorem 6.7, we consider the extreme copositive matrices

$$A_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{28}$$

Let $t_1, t_2 \geq 0$. The matrix $t_1 A_1 + t_2 A_2$ belongs to $\partial\mathcal{C}_2$ because its smallest Pareto eigenvalue is equal to 0. Indeed,

$$\Pi\left(\begin{bmatrix} t_1 & t_2 \\ t_2 & 0 \end{bmatrix}\right) = \left\{0,\, t_1,\, \frac{t_1 + \sqrt{t_1^2 + 4t_2^2}}{2}\right\}.$$

For $n \geq 3$, one just needs to enlarge the matrices in (28) by filling with zeros. □

6.4 Metric projection onto $\mathcal{C}_n$

How far is an arbitrary matrix $A \in \mathbb{S}_n$ from being copositive? Rigorously speaking, this question is about measuring the distance

$$\text{dist}[A, \mathcal{C}_n] = \inf_{X \in \mathcal{C}_n} \|A - X\| \tag{29}$$

from A to the closed convex cone $\mathcal{C}_n$. Here, $\|\cdot\|$ refers to the norm associated with the trace inner product. Given the Euclidean nature of the normed space $(\mathbb{S}_n, \|\cdot\|)$, the minimization problem (29) admits a unique solution, denoted by $\text{proj}[A, \mathcal{C}_n]$ and called the metric projection of A onto $\mathcal{C}_n$.

Thanks to Moreau's decomposition theorem [84], any matrix $A \in \mathbb{S}_n$ can be decomposed in the form

$$A = \text{proj}[A, \mathcal{C}_n] + \text{proj}[A, -\mathcal{G}_n] \tag{30}$$

with

$$-\mathcal{G}_n = \{B \in \mathbb{S}_n : \langle A, B\rangle \leq 0 \text{ for all } A \in \mathcal{C}_n\} \tag{31}$$

standing for the "polar" cone of $\mathcal{C}_n$. We use the notation $-\mathcal{G}_n$ because the set on the right-hand side of (31) is simply the opposite of the dual cone $\mathcal{G}_n$. Sometimes one refers to $-\mathcal{G}_n$ as the cone of completely negative matrices. Since the projections

$$A^{\text{cop}} := \text{proj}[A, \mathcal{C}_n], \quad A^{\text{cn}} := \text{proj}[A, -\mathcal{G}_n] \tag{32}$$

are mutually orthogonal matrices in the Euclidean space $(\mathbb{S}_n, \langle\cdot,\cdot\rangle)$, the decomposition (30) yields the Pythagorean law

$$(\mathrm{dist}[A, \mathcal{C}_n])^2 + (\mathrm{dist}[A, -\mathcal{G}_n])^2 = \|A\|^2.$$

So, if one wishes, one can shift the attention from (29) to the minimal distance problem

$$\mathrm{dist}[A, -\mathcal{G}_n] = \inf_{Y \in -\mathcal{G}_n} \|A - Y\|. \tag{33}$$

Even better, one can work with (29) and (33) in tandem.

To the best of our knowledge, nobody has obtained so far an explicit formula for either one of the projections mentioned in (32). Due to the difficulty of the problem, we shall not attempt here to obtain explicit characterizations for such projections. We shall not even try to derive exact estimates for the terms $\mathrm{dist}[A, \mathcal{C}_n]$ and $\mathrm{dist}[A, -\mathcal{G}_n]$. The next upper bound for $\mathrm{dist}[A, \mathcal{C}_n]$ is coarse in general, but it has the merit of being easily computable.

Proposition 6.10. *For any $A \in \mathbb{S}_n$, one has*

$$\mathrm{dist}[A, \mathcal{C}_n] \leq \min\{\mathrm{dist}[A, \mathcal{N}_n],\, \mathrm{dist}[A, \mathcal{P}_n]\}. \tag{34}$$

The terms in the above minimum can be evaluated with the help of the formulas

$$\mathrm{dist}[A, \mathcal{N}_n] = \left[\sum_{i,j=1}^{n} \left(\min\{a_{i,j}, 0\}\right)^2\right]^{1/2}, \tag{35}$$

$$\mathrm{dist}[A, \mathcal{P}_n] = \left[\sum_{i=1}^{n} \left(\min\{\lambda_i(A), 0\}\right)^2\right]^{1/2}, \tag{36}$$

where $\lambda_1(A), \ldots, \lambda_n(A)$ are the eigenvalues of A.

Proof. The inequality (34) is a direct consequence of the inclusion $\mathcal{N}_n \cup \mathcal{P}_n \subset \mathcal{C}_n$. The equality (35) is obvious. Formula (36) is known or ought to be known. A sketch of the proof runs as follows: first of all, observe that $\mathcal{P}_n$ is *unitarily invariant* in the sense that

$$A \in \mathcal{P}_n \quad \Longrightarrow \quad U^T A U \in \mathcal{P}_n \quad \text{for all } U \in \mathcal{O}_n$$

with $\mathcal{O}_n$ denoting the group of orthogonal matrices of order n. By relying on the Commutation Principle [61, Lemma 4] for variational problems with unitarily invariant data, one obtains the reduction formula

$$\mathrm{dist}[A, \mathcal{P}_n] = \mathrm{dist}[\lambda(A), \mathbb{R}^n_+], \tag{37}$$

where $\lambda(A) = (\lambda_1(A), \ldots, \lambda_n(A))^T$ denotes the vector of eigenvalues of A. For avoiding any ambiguity in the definition of $\lambda(A)$, we arrange the eigenvalues of A in a nondecreasing order, *i.e.*, from $\lambda_1(A) = \lambda_{\min}(A)$ to $\lambda_n(A) = \lambda_{\max}(A)$. The choice of the ordering mechanism is not essential because $\mathbb{R}^n_+$ is permutation invariant. By working out the right-hand side of (37), one readily gets the announced characterization of $\mathrm{dist}[A, \mathcal{P}_n]$. □

One should not be overly optimistic concerning Proposition 6.10. The relation (34) can be written as an equality when $n = 2$, but starting from $n = 3$ the situation can deteriorate dramatically. It is not difficult to construct a copositive matrix such that the upper bound (34) is as large as one wishes. To see this, just form the matrix

$$A = \begin{bmatrix} t & -t & 0 \\ -t & t & t \\ 0 & t & 0 \end{bmatrix} = \underbrace{\begin{bmatrix} t & -t & 0 \\ -t & t & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{in\ \mathcal{P}_3} + \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & t \\ 0 & t & 0 \end{bmatrix}}_{in\ \mathcal{N}_3}$$

and let the positive parameter t go to ∞. The degeneracy phenomenon pointed out in the above lines is not surprising altogether. We knew already that the usual spectrum of a symmetric matrix is not a proper mathematical tool for dealing with copositivity issues. The following result is a Hoffman-type upper estimate for $\mathrm{dist}[A, \mathcal{C}_n]$ that can be derived by using the theory of Pareto spectra.

Proposition 6.11. *For any $A \in \mathbb{S}_n$, one has*

$$\mathrm{dist}[A, \mathcal{C}_n] \leq \sqrt{n}\ [\mu(A)]^-, \tag{38}$$

where $a^- = \max\{-a, 0\}$ stands for the negative part of $a \in \mathbb{R}$.

Proof. One may suppose that A is not copositive, otherwise each side of (38) is equal to zero. As pointed out in [90, Proposition 2], Pareto spectra obey the translation rule

$$\Pi(A - tI_n) = \Pi(A) - t \tag{39}$$

for all $t \in \mathbb{R}$. In view of (39) and Theorem 4.3, the shifted matrix $A - \mu(A)I_n$ is copositive. Hence,

$$\mathrm{dist}[A, \mathcal{C}_n] \leq \|A - (A - \mu(A)I_n)\| = -\sqrt{n}\,\mu(A).$$

Note, incidentally, that the right-hand side of (38) is always nonnegative. □

For seeing that $\sqrt{n}$ is the smallest possible factor in front of $[\mu(A)]^-$, consider the example

$$A = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}, \quad A^{\mathrm{cop}} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

The matrix A^{cop} is obtained by exploiting Moreau's theorem. One gets in this case $\mathrm{dist}[A, \mathcal{C}_2] = \sqrt{2}$ and $\mu(A) = -1$. However, the inequality (38) is not meant to be sharp. We mention this upper bound just to show an interesting application of the coefficient $\mu(A)$. In the same vein as in Proposition 6.11, one can write also

$$\mathrm{dist}[A, \mathcal{C}_n] \leq n\ [\gamma(A)]^-. \tag{40}$$

The key observation for obtaining the upper estimate (40) is that $A - \gamma(A)\mathbf{1_n}\mathbf{1_n}^T$ is copositive thanks to Proposition 5.1. The inequality (40) is less interesting than (38), just because the factor n is worse than $\sqrt{n}$.

Remark 6.12. For each $p \in \{1, \ldots, n\}$, consider the positively homogeneous concave function

$$A \in \mathbb{S}_n \mapsto g_p(A) = \text{sum of the } p \text{ smallest eigenvalues of } A$$

and the corresponding closed convex cone

$$\mathcal{K}_{p,n} = \{A \in \mathbb{S}_n : g_p(A) \geq 0\}. \tag{41}$$

Clearly, $\mathcal{K}_{1,n} \subset \mathcal{K}_{2,n} \subset \ldots \subset \mathcal{K}_{n,n}$. Also $\mathcal{C}_n$ is sandwiched between $\mathcal{K}_{1,n} = \mathcal{P}_n$ and the half-space $\mathcal{K}_{n,n} = \{A \in \mathbb{S}_n : \mathrm{tr}(A) \geq 0\}$, like all the $\mathcal{K}_{p,n}$ $(p = 2, \ldots, n-1)$; however there is no direct comparison between such $\mathcal{K}_{p,n}$ and $\mathcal{C}_n$. By the way, the sets defined by (41) are unitarily invariant, but $\mathcal{C}_n$ is not. From a complexity point of view, this is a substantial difference. Formula (38) is close in spirit to the Hoffman-type estimate

$$\mathrm{dist}[A, \mathcal{K}_{p,n}] \leq \sqrt{n} \left[\frac{g_p(A)}{p}\right]^- \tag{42}$$

derived by Azé and Hiriart-Urruty [3, Theorem 2.1]. The shortest possible way to prove this inequality is by observing that $A - (g_p(A)/p)\, I_n \in \mathcal{K}_{p,n}$, a relation that explains why the eigenvalues $\lambda_1(A), \ldots, \lambda_p(A)$ must be averaged in (42).

6.5 Angular structure of $\mathcal{C}_n$

As mentioned in Proposition 1.2, the convex cone $\mathcal{C}_n$ contains both $\mathcal{P}_n$ and $\mathcal{N}_n$. How big is $\mathcal{C}_n$ after all? There are different coefficients that serve to measure the size of a convex cone, one of them being the so-called maximal angle. By definition, the maximal angle of $\mathcal{C}_n$ is the largest angle that can be formed with a pair of unit vectors taken from $\mathcal{C}_n$. In short,

$$\theta_{\max}(\mathcal{C}_n) = \max_{\substack{X,Y \in \mathcal{C}_n \\ \|X\|=1, \|Y\|=1}} \arccos\langle X, Y\rangle. \tag{43}$$

If X and Y are matrices solving (43), then (X, Y) is called an *antipodal pair* of $\mathcal{C}_n$.

In order to avoid the bothersome inverse cosinus operation, it is convenient sometimes to write the angle maximization problem (43) in the equivalent form

$$\cos[\theta_{\max}(\mathcal{C}_n)] = \min_{\substack{X,Y \in \mathcal{C}_n \\ \|X\|=1, \|Y\|=1}} \langle X, Y\rangle. \tag{44}$$

Despite its simple appearence, the nonconvex minimization problem (44) is quite tricky.

The concept of minimal angle is also of importance, but it takes longer to introduce and it is not so easy to apprehend. The first thing one has to do is write down the optimality conditions for the minimization problem (44). One gets in this way a combination of feasibility conditions

$$X \in C_n,\ Y \in \mathcal{C}_n, \tag{45}$$

$$\|X\| = 1,\ \|X\| = 1, \tag{46}$$

plus criticality (or stationarity) conditions

$$Y - \langle X, Y\rangle X \in \mathcal{G}_n, \tag{47}$$

$$X - \langle X, Y\rangle Y \in \mathcal{G}_n. \tag{48}$$

Feasibility and criticality are both necessary, but not sufficient, for antipodality.

Definition 6.13. *If $X, Y \in \mathbb{S}_n$ are distinct matrices satisfying the system (45)-(48), then one says that (X, Y) is a critical pair of $\mathcal{C}_n$. The angular spectrum of $\mathcal{C}_n$ is defined as the set*

$$\Omega(\mathcal{C}_n) = \{\arccos\langle X, Y\rangle : (X, Y) \text{ is a critical pair of } \mathcal{C}_n\}. \tag{49}$$

Each element of (49) is called a critical angle of $\mathcal{C}_n$. The smallest element of (49), denoted by $\theta_{\min}(\mathcal{C}_n)$, is called the minimal angle of $\mathcal{C}_n$.

The notation for the minimal angle is consistent with the corresponding one for the maximal angle. Indeed, one has

$$\begin{aligned} \theta_{\min}(\mathcal{C}_n) &= \min\{\theta : \theta \in \Omega(\mathcal{C}_n)\}, \\ \theta_{\max}(\mathcal{C}_n) &= \max\{\theta : \theta \in \Omega(\mathcal{C}_n)\}. \end{aligned}$$

Angular spectra of general convex cones have been studied in depth by Iusem and Seeger in a series of papers [59, 61, 62, 64]. Here we concentrate on the specific case of $\mathcal{C}_n$. The angle maximization problem

$$\theta_{\max}(\mathcal{G}_n) = \max_{\substack{U,V \in \mathcal{G}_n \\ \|U\|=1, \|V\|=1}} \arccos\langle U, V\rangle, \tag{50}$$

relative to the dual cone $\mathcal{G}_n$ can be treated in the same manner. The feasibility-criticality system associated with (50) is

$$\begin{aligned} U \in \mathcal{G}_n,\ V \in \mathcal{G}_n, \\ \|U\| = 1,\ \|V\| = 1, \\ V - \langle U, V\rangle U \in \mathcal{C}_n, \\ U - \langle U, V\rangle V \in \mathcal{C}_n, \end{aligned}$$

and with such an ingredient one can define the angular spectrum of $\mathcal{G}_n$.

As a particular instance of a general duality result established in [64, Theorem 3], one has

$$\begin{aligned} \Omega(\mathcal{G}_n) &= \{\pi - \theta : \theta \in \Omega(\mathcal{C}_n)\}, \\ \Omega(\mathcal{C}_n) &= \{\pi - \theta : \theta \in \Omega(\mathcal{G}_n)\}. \end{aligned}$$

Hence, up to a reflexion, the cones $\mathcal{C}_n$ and $\mathcal{G}_n$ have the same angular structure. Observe also that

$$\begin{aligned} \theta_{\min}(\mathcal{C}_n) + \theta_{\max}(\mathcal{G}_n) &= \pi, \\ \theta_{\min}(\mathcal{G}_n) + \theta_{\max}(\mathcal{C}_n) &= \pi. \end{aligned} \tag{51}$$

By exploiting the equality (51), one easily gets:

Proposition 6.14. *For all $n \geq 2$, one has $\theta_{\min}(\mathcal{C}_n) = \pi/2$. Furthermore, (X, Y) is a critical pair forming the angle $\pi/2$ if and only if $X, Y \in \mathbb{S}_n$ are completely positive, of unit length, and such that $X_{i,j}Y_{i,j} = 0$ for all $i, j \in \{1, \ldots, n\}$.*

Proof. Clearly, $\theta_{\max}(\mathcal{G}_n) \leq \theta_{\max}(\mathcal{P}_n) \leq \pi/2$. On the other hand, if e_1 and e_2 denote the first two canonical vectors of $\mathbb{R}^n$, then the matrices $e_1e_1^T$ and $e_2e_2^T$ are completely positive, of unit length, and such that $\langle e_1e_1^T, e_2e_2^T\rangle = 0$. This shows that $\theta_{\max}(\mathcal{G}_n) = \theta_{\max}(\mathcal{P}_n) = \pi/2$. Hence,

$$\theta_{\min}(\mathcal{C}_n) = \pi - \theta_{\max}(\mathcal{G}_n) = \pi - \pi/2 = \pi/2.$$

Let (X, Y) be a critical pair achieving the minimal angle of $\mathcal{C}_n$. Since X and Y are orthogonal, the criticality conditions (47)-(48) force X and Y to be completely positive. In particular, X and Y are nonnegative entrywise, and $X_{i,j}Y_{i,j} = 0$ for all $i, j \in \{1, \ldots, n\}$. □

Computing the maximal angle of $\mathcal{C}_n$ is a more delicate matter. The analysis of the two-dimensional case is as follows.

Proposition 6.15. *The maximal angle of $\mathcal{C}_2$ is $3\pi/4$. Furthermore, the pair*

$$\widehat{X} = \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{bmatrix}, \quad \widehat{Y} = \begin{bmatrix} 0 & \sqrt{2}/2 \\ \sqrt{2}/2 & 0 \end{bmatrix} \tag{52}$$

is the only one that achieves this angle.

Proof. As observed in [64], the copositive matrices $\widehat{X}$ and $\widehat{Y}$ have unit length and form an angle equal to $3\pi/4$. So, one knows already that $\theta_{\max}(\mathcal{C}_2) \geq 3\pi/4$. For proving that (52) is the unique antipodal pair of $\mathcal{C}_2$, we write

$$X = \begin{bmatrix} a & b \\ b & c \end{bmatrix}, \quad Y = \begin{bmatrix} d & e \\ e & f \end{bmatrix}$$

and solve the variational problem

$$\cos\left[\theta_{\max}(\mathcal{C}_2)\right] = \min_{\substack{a,b,c \\ d,e,f}} (ad + 2be + cf), \tag{53}$$

where the minimization variables are restricted to the normalization constraints

$$a^2 + 2b^2 + c^2 = 1, \tag{54}$$

$$d^2 + 2e^2 + f^2 = 1, \tag{55}$$

and the copositivity ones

$$\begin{aligned} b + \sqrt{ac} &\geq 0, \\ e + \sqrt{df} &\geq 0, \\ a \geq 0, c \geq 0, d \geq 0, f &\geq 0. \end{aligned}$$

It is clear that b and e must be chosen of opposite signs. We take, for instance, $b \leq 0$ and $e \geq 0$. In such a case, the copositivity constraints take the simpler form

$$\begin{aligned} ac - b^2 &\geq 0, \\ b &\leq 0, \\ a \geq 0, c \geq 0, d \geq 0, f \geq 0, e &\geq 0. \end{aligned} \tag{56}$$

Next, one observes that the best strategy consists in taking e as large as possible and, at the same time, d and f as small as possible. This observation and (55) lead to $d = 0, f = 0$ and $e = \sqrt{2}/2$. This explains the form of $\widehat{Y}$. Plugging this information into (53), one gets the smaller size problem

$$\cos\left[\theta_{\max}(\mathcal{C}_2)\right] = \min_{a,b,c} \sqrt{2}\, b, \tag{57}$$

where the variables $a \geq 0, c \geq 0, b \leq 0$ are restricted to (54) and (56). One can easily check that $(a, b, c) = (1/2, -1/2, 1/2)$ is the unique solution to (57). This explains the form of $\widehat{X}$. □

Remark 6.16. The matrices $\widehat{X}$ and $\widehat{Y}$ given by (52) belong to $\partial\mathcal{C}_2$. This is consistent with the general theory of critical pairs in convex cones. By contrast, what is more specific to the case of $\mathcal{C}_2$ is that $\widehat{X}$ and $\widehat{Y}$ are extreme copositive matrices.

It is not clear to us how to derive an explicit formula for $\theta_{\max}(\mathcal{C}_n)$ when $n \geq 3$. This question will have to be left open for the time being. We are aware, however, that the sequence $\{\theta_{\max}(\mathcal{C}_n)\}_{n\geq 2}$ behaves monotonically.

Proposition 6.17. *For all $n \geq 2$, one can write the inclusion $\Omega(\mathcal{C}_n) \subset \Omega(\mathcal{C}_{n+1})$ and, in particular, the inequality $\theta_{\max}(\mathcal{C}_n) \leq \theta_{\max}(\mathcal{C}_{n+1})$.*

Proof. Let $\theta \in \Omega(\mathcal{C}_n)$. Then, $\theta = \arccos\langle X, Y\rangle$ corresponds to the angle formed by some critical pair (X, Y) of $\mathcal{C}_n$. The matrices

$$X' = \begin{bmatrix} X & 0 \\ 0 & 0 \end{bmatrix}, \quad Y' = \begin{bmatrix} Y & 0 \\ 0 & 0 \end{bmatrix}$$

of order $n+1$ have unit length and belong to $\mathcal{C}_{n+1}$. Furthermore,

$$Y' - \langle X', Y'\rangle X' = Y' - \langle X, Y\rangle X' = \begin{bmatrix} Y - \langle X, Y\rangle X & 0 \\ 0 & 0 \end{bmatrix} \in \mathcal{G}_{n+1}.$$

Similarly, $X' - \langle X', Y'\rangle Y' \in \mathcal{G}_{n+1}$. In short, (X', Y') is a critical pair of $\mathcal{C}_{n+1}$, and

$$\theta = \arccos\langle X, Y\rangle = \arccos\langle X', Y'\rangle \in \Omega(\mathcal{C}_{n+1}).$$

This completes the proof of the announced inclusion. The upward monotonicity of $\{\theta_{\max}(\mathcal{C}_n)\}_{n\geq 2}$ is then obtained by taking the supremum on each side of the inclusion. □

Remark 6.18. Intensive numerical experimentation with randomly generated pairs of copositive matrices of order 3 has shown that

$$\widehat{X} = \begin{bmatrix} 1/2 & -1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \widehat{Y} = \begin{bmatrix} 0 & \sqrt{2}/2 & 0 \\ \sqrt{2}/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

is a strong candidate as antipodal pair of $\mathcal{C}_3$. From here, this is only one step to conjecture that $\theta_{\max}(\mathcal{C}_n) = 3\pi/4$ for all $n \geq 2$. It is quite bothersome, but we do not have yet a serious argument for proving (or disproving) this conjecture.

6.6 Degree of solidity of $\mathcal{C}_n$

Recall that a convex set in a normed vector space is said to be *solid* if its interior is nonempty. There are several ways of measuring the degree of solidity of a closed convex cone in a given Euclidean space. A large variety of solidity indices have been introduced and studied by Iusem and Seeger [58, 60, 63]. For instance, the "angular" solidity index of a closed convex cone K is defined by

$$\mathcal{S}_{\text{ang}}(K) = \sin\left(\frac{\theta_{\min}(K)}{2}\right).$$

Another interesting choice is the so-called Frobenius solidity index, whose definition is

$$\mathcal{S}_{\text{frob}}(K) = \sup_{\substack{z\in K\\ \|z\|=1}} \operatorname{dist}[z, \partial K]. \tag{58}$$

Freund and collaborators [39, 42, 43] refer to (58) as the width of K, but we shall not follow this terminology because it also has another meaning in convex analysis.

Concerning the specific case of the cone $\mathcal{C}_n$, its angular solidity index is trivial to evaluate. In view of Proposition 6.14, one knows already that:

Corollary 6.19. $\mathcal{S}_{\text{ang}}(\mathcal{C}_n) = \sqrt{2}/2$ *for all* $n \geq 2$.

A little bit more difficult is estimating the expression

$$\mathcal{S}_{\text{frob}}(\mathcal{C}_n) = \sup_{\substack{Z\in \mathcal{C}_n\\ \|Z\|=1}} \operatorname{dist}[Z, \partial \mathcal{C}_n], \tag{59}$$

or, equivalently,

$$\mathcal{S}_{\text{frob}}(\mathcal{C}_n) = \sup\{r : \|Z\| = 1, r \geq 0,\, \mathbb{B}_r(Z) \subset \mathcal{C}_n\} \tag{60}$$

with $\mathbb{B}_r(Z)$ denoting the closed ball of center Z and radius r. According to the latter formulation, the term $\mathcal{S}_{\text{frob}}(\mathcal{C}_n)$ corresponds to the radius of the largest closed ball centered at a unit matrix and contained in $\mathcal{C}_n$. Indeed, the radius maximization problem (60) has a unique solution, say (Z_n, r_n), and

$$\begin{aligned} \mathcal{S}_{\text{frob}}(\mathcal{C}_n) &= r_n \\ &= \sup\{r : r \geq 0,\, \mathbb{B}_r(Z_n) \subset \mathcal{C}_n\}. \end{aligned}$$

The center Z_n of the largest ball is, of course, the unique solution to (59). For convenience, we refer to Z_n as the *metric center* of $\mathcal{C}_n$. Geometrically speaking, the half-line generated by the metric center can be seen as a sort of central axis of $\mathcal{C}_n$. Parenthetically, the existence and uniqueness of the metric center is not exclusive of $\mathcal{C}_n$, but it concerns any nontrivial solid closed convex cone in an Euclidean space.

Proposition 6.20. *For all* $n \geq 2$, *the metric center of* $\mathcal{C}_n$ *is the normalized identity matrix* $\widehat{I}_n = \frac{1}{\sqrt{n}} I_n$. *Furthermore,* $\mathcal{S}_{\text{frob}}(\mathcal{C}_n) = 1/\sqrt{n}$.

Proof. As a particular instance of [58, Proposition 6.3], one can write

$$\mathcal{S}_{\text{frob}}(\mathcal{C}_n) = \inf_{B\in \operatorname{co}[\mathcal{G}_n \cap \Sigma_n]} \|B\|$$

with Σ_n standing for the unit sphere in $\mathbb{S}_n$. Let $\{e_1, \ldots, e_n\}$ denote the canonical basis of $\mathbb{R}^n$. Since

$$\frac{1}{n} I_n = \frac{1}{n} e_1 e_1^T + \ldots + \frac{1}{n} e_n e_n^T$$

is a convex combination of matrices in $\mathcal{G}_n \cap \Sigma_n$, one has

$$\mathcal{S}_{\text{frob}}(\mathcal{C}_n) \leq \|(1/n) I_n\| = 1/\sqrt{n}\,.$$

On the other hand, it can be shown that the ball

$$\left\{A \in \mathbb{S}_n : \left\|A - \widehat{I}_n\right\| \leq 1/\sqrt{n}\right\}$$

is contained in the cone $\mathcal{P}_n$, which in turn is contained in $\mathcal{C}_n$. It follows that

$$1/\sqrt{n} \leq \mathcal{S}_{\text{frob}}(\mathcal{P}_n) \leq \mathcal{S}_{\text{frob}}(\mathcal{C}_n).$$

In this way, we have proven that

$$\mathcal{S}_{\text{frob}}(\mathcal{C}_n) = \mathcal{S}_{\text{frob}}(\mathcal{P}_n) = 1/\sqrt{n}.$$

Let Z be the metric center of $\mathcal{C}_n$. One necessarily has

$$\min\{Z_{1,1}, \ldots, Z_{n,n}\} \geq 1/\sqrt{n}, \tag{61}$$

otherwise the ball $B_{1/\sqrt{n}}(Z)$ touches the exterior of $\mathcal{C}_n$ (recall that the diagonal entries of a copositive matrix are nonnegative). Since Z has unit length, the requirement (61) forces Z to be equal to $\widehat{I}_n$. □

Remark 6.21. A closer inspection of the above proof reveals that Proposition 6.20 is not specific to $\mathcal{C}_n$, but it applies to any closed convex cone lying between $\mathcal{P}_n$ and $\{A \in \mathbb{S}_n : a_{1,1} \geq 0, \ldots, a_{n,n} \geq 0\}$.

The following corollary concerning the asymptotic behavior of the sequence $\{\mathcal{S}_{\text{frob}}(\mathcal{C}_n)\}_{n\geq 2}$ is somehow against intuition: despite the fact that $\mathcal{C}_n$ has a large minimal angle, its Frobenius index of solidity is rather small.

Corollary 6.22. *$\mathcal{C}_n$ loses solidity in the Frobenius sense as the dimension n increases. More precisely,* $\lim_{n\to\infty} \mathcal{S}_{\text{frob}}(\mathcal{C}_n) = 0$.

7 Selected topics related to copositivity

7.1 Copositivity with respect to a polyhedral cone

Recall that copositivity of $A \in \mathbb{S}_n$ relative to a closed convex cone K refers to the property

$$x^T A x \geq 0 \quad \text{for all } x \in K. \tag{62}$$

If the cone K is polyhedral, then one can represent it in the form $K = \{Gz : z \in \mathbb{R}^p_+\}$, where G stands for a real matrix whose columns $\{g_1, \ldots, g_p\}$ are positively linearly independent vectors in $\mathbb{R}^n$. In such a case, the condition (62) takes the form

$$z^T G^T A G z \geq 0 \quad \text{for all } z \in \mathbb{R}^p_+.$$

This corresponds to the usual notion of copositivity applied to the matrix $G^T A G \in \mathbb{S}_p$, so we are back to a well known framework. In most applications, hovever, p is much larger than n. That copositivity with respect to a polyhedral cone can be converted into usual copositivity has been observed by a number of authors (*cf.* [11, 38]).

The concept of copositivity with respect to a polyhedral cone has many applications. For instance, it enters into the picture when it comes to write down a second-order local optimality condition for the minimization of a quadratic function on a polyhedral set:

$$\min_{x\in\Omega}\left\{b^Tx+\frac{1}{2}\,x^TAx\right\}. \tag{63}$$

The next theorem by Contesse [26, Theorem 1] shows elegantly the role of copositivity in this matter. Other results in the same vein can be found in [12, 13, 33]. The notation $T_\Omega(\bar{x})$ refers to the tangent cone to Ω at $\bar{x}$.

Theorem 7.1. *Let $A\in\mathbb{S}_n$ and Ω be a polyhedral set in $\mathbb{R}^n$. Then, $\bar{x}\in\Omega$ is a local solution to (63) if and only if*

(a) $(A\bar{x}+b)^Th\geq 0$ for all $h\in T_\Omega(\bar{x})$, and

(b) A is copositive with respect to the polyhedral cone $K=\{h\in T_\Omega(\bar{x}):(A\bar{x}+b)^Th=0\}$.

7.2 Copositivity and linear complementarity

The standard linear complementarity problem consists in finding a solution $x\in\mathbb{R}^n$ to the system

$$x\geq 0,\quad Ax+b\geq 0,\quad x^T(Ax+b)=0. \tag{64}$$

There is a good dozen of books and surveys devoted to this specific equilibrium model, so we do not need to indulge in lengthy explanations. The vector $b\in\mathbb{R}^n$ is usually viewed as a parameter. The problem (64) makes sense for a general $n\times n$ real matrix A, but we concentrate only on the symmetric case.

Under symmetry, the system (64) corresponds to the stationary point problem associated to the linear-quadratic program

$$v(A,b)=\inf_{x\geq 0}\left\{b^Tx+\frac{1}{2}\,x^TAx\right\}. \tag{65}$$

A particular version of the celebrated Frank-Wolfe theorem asserts that (65) is solvable if and only if the infimal value $v(A,b)$ is finite. The next proposition explains the role of copositivity in connection with this issue.

Proposition 7.2. *For $A\in\mathbb{S}_n$, the following statements are equivalent:*

(a) A is copositive (respectively, strictly copositive).

(b) for all $b\in\mathbb{R}^n_+$ (respectively, for all $b\in\mathbb{R}^n$), the quadratic function

$$x\in\mathbb{R}^n\mapsto f(x)=b^Tx+\frac{1}{2}\,x^TAx$$

is bounded from below on $\mathbb{R}^n_+$.

As one can see, the difference between copositivity and strict copositivity is subtle, but it has a profound impact on the solvability of linear-quadratic programs. More specialized applications of copositivity in the realm of linear complementarity can be found in [69] or in Section 2.5 of the book [40].

7.3 Probabilistic considerations concerning copositivity

If $E \in \mathbb{S}_n$ is a nonzero matrix, then $\{X \in \mathbb{S}_n : \langle E, X\rangle \geq 0\}$ is a half-space in $\mathbb{S}_n$. As indicated by its name, such a set fills half of the space $\mathbb{S}_n$. The room occupied by the cone $\mathcal{N}_n$ is only $2^{-n(n+1)/2}$ of the space of $\mathbb{S}_n$. Recall that $\mathcal{G}_n$ is contained in $\mathcal{N}_n$. Hence, when n is large, $\mathcal{G}_n$ fills an incredibly small portion of $\mathbb{S}_n$.

From a measure theoretic point of view, also the size of $\mathcal{C}_n$ is very small. This can be better explained by using the concept of normalized volume studied in [47]. The fact that $\mathcal{C}_n$ fills only a small portion of $\mathbb{S}_n$ should not be so surprising after all. To see this, just think of the low dimensional case $n = 3$, in which already 7 inequalities must be fulfilled in order to qualify for copositivity. Contrarily to popular belief, joining the elite of copositive matrices is a tough job!

Thanks to [47, Proposition 5], evaluating the normalized volume of a closed convex cone K in some Euclidean space, say $\mathbb{R}^d$, amounts to computing

$$P[\mathbf{x} \in K] \equiv \text{probability that } \mathbf{x} \text{ falls in } K,$$

where $\mathbf{x}$ is a d-dimensional random vector with a spherically symmetric distribution law. For all practical purposes, think of $\mathbf{x}$ as a Gaussian vector, *i.e.*, normally distributed with the origin as mathematical expectation and with the identity matrix as covariance matrix. We shall not recall here the concept of normalized volume, but we shall explain the smallness of $\mathcal{C}_n$ by using the formalism of probability theory.

Suppose that $\mathbf{A}$ is a Gaussian random matrix in $\mathbb{S}_n$, meaning that

- the entries $\mathbf{a_{i,j}}$ (with $i, j \in \{1, \ldots, n\}, i \leq j$) are stochastically independent random variables with standard normal distribution, and
- the lower triangular part of $\mathbf{A}$ is a copy of its upper triangular part, so as to get a symmetric matrix.

The problem at hand is that of evaluating the probability $p_n = P[\mathbf{A} \in \mathcal{C}_n]$. If this number is small, then one can legitimely say that $\mathcal{C}_n$ fills a small portion of the space $\mathbb{S}_n$. Unfortunately, obtaining an explicit and easily computable formula for p_n is a task beyond reach. Already the case $n = 2$ is relatively nasty.

Proposition 7.3. *Let $\Phi : \mathbb{R} \to [0, 1]$ be the cumulative distribution function of the standard normal law. Then,*

$$p_2 = \frac{1}{4} - \frac{1}{2\pi} \int_0^\infty \int_0^\infty \Phi(-\sqrt{t_1 t_2})\, e^{-\frac{1}{2}(t_1^2+t_2^2)}\, dt_1 dt_2 \;\approx 0.1829.$$

Proof. In view of Proposition 2.1 and the Gaussian character of $\mathbf{A}$, one just needs to simplify the triple integral

$$p_2 = \int_\Omega \left(\frac{1}{\sqrt{2\pi}}\right)^3 \; e^{-\frac{1}{2}(t_1^2+t_2^2+t_3^2)}\, dt_1 dt_2 dt_3,$$

where integration takes place over the region $\Omega = \{t \in \mathbb{R}^3 : t_1 \geq 0, t_2 \geq 0, t_3 + \sqrt{t_1 t_2} \geq 0\}$. In fact, the only thing one can do explicitly is carrying out the integration with respect to t_3. The approximated value of p_2 can be obtained by numerical integration of the double integral. For avoiding cumbersome numerical work, we just used Monte Carlo simulation with a sample of 10^8 Gaussian random matrices in $\mathbb{S}_2$. □

As far as the case $n = 3$ is concerned, one readily sees that $p_3 \leq 1/8$. This crude upper bound is obtained by neglecting all the copositivity constraints, except for the nonnegativity of the diagonal entries. Monte Carlo simulation[3] with a sample of 10^8 Gaussian random matrices in $\mathbb{S}_3$ gave the estimation $p_3 \approx 0.0496$. Roughly speaking, only 1 out of 20 matrices in $\mathbb{S}_3$ turned out to be copositive.

Remark 7.4. When n increases, the number of copositivity constraints increases as well. That

$$P[\mathbf{A} \in \mathcal{N}_n] = \left(\frac{1}{2}\right)^{n(n+1)/2} \leq p_n \leq \left(\frac{1}{2}\right)^n$$

is clear, but there are good reasons to conjecture that p_n goes to 0 much faster than $(1/2)^n$. In fact, one has the sharpening

$$p_n \leq p_{\lfloor n/2 \rfloor} p_{n-\lfloor n/2 \rfloor} \leq (1/2)^n,$$

and there is still room for improvement. Here, $\lfloor n/2 \rfloor$ denotes the lower integer part of $n/2$.

We end this section by addressing a question raised by one of the referees. Suppose that one cuts $\mathcal{C}_n$ with a prescribed affine hyperplane in order to produce a compact convex set, say

$$\mathcal{C}_n^E = \{X \in \mathcal{C}_n : \langle E, X \rangle = 1\}. \tag{66}$$

Is it possible to derive an estimate for the relative Lebesgue measure of this set? The next result is obtained by relying on the Brunn-Minkowski inequality. The symbols $\mathcal{P}_n^E$ and $\mathcal{N}_n^E$ are defined as in (66).

Proposition 7.5. *Let $E \in \mathrm{int}(\mathcal{G}_n)$ and $\mathrm{meas}(\,\cdot\,)$ be the Lebesgue measure on the affine hyperplane defined by E. Then,*

$$\left[\mathrm{meas}(\mathcal{P}_n^E)\right]^{1/d} + \left[\mathrm{meas}(\mathcal{N}_n^E)\right]^{1/d} \leq 2\left[\mathrm{meas}(\mathcal{C}_n^E)\right]^{1/d}$$

with $d + 1 = n(n+1)/2$.

Proof. Since E belongs to the interior of $\mathcal{G}_n$, the set $\mathcal{C}_n^E$ is compact. Due to Proposition 1.2, also $\mathcal{P}_n^E$ and $\mathcal{N}_n^E$ are compact, and one has

$$(1/2)\,\mathcal{P}_n^E + (1/2)\,\mathcal{N}_n^E \subset (\mathcal{P}_n + \mathcal{N}_n)^E \subset \mathcal{C}_n^E.$$

Since d is equal to the dimension of the affine hyperplane $\{X \in \mathbb{S}_n : \langle E, X \rangle = 1\}$, the Brunn-Minkowski inequality tells us that the function $[\mathrm{meas}(\,\cdot\,)]^{1/d}$ is concave. Hence,

$$\begin{aligned}(1/2)\left[\mathrm{meas}(\mathcal{P}_n^E)\right]^{1/d} + (1/2)\left[\mathrm{meas}(\mathcal{N}_n^E)\right]^{1/d} &\leq \left[\mathrm{meas}\left((1/2)\,\mathcal{P}_n^E + (1/2)\,\mathcal{N}_n^E\right)\right]^{1/d} \\ &\leq \left[\mathrm{meas}(\mathcal{C}_n^E)\right]^{1/d}.\end{aligned}$$

This completes the proof. □

[3]We thank our colleague D. Gourion (Avignon) for the computer implementation and numerical testing with randomly generated data.

7.4 Copositivity and invertibility

The inverse A^{-1} of a positive definite matrix $A \in \mathbb{S}_n$ is again positive definite. Now, suppose that $A \in \mathbb{S}_n$ is nonsingular and copositive. What can be said about A^{-1}? There are not too many results on inverses of copositive matrices. To start, it should be mentioned that copositivity is not preserved by inversion.

Example 7.6. Consider the 2×2 matrices

$$A = \begin{bmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 1 \end{bmatrix}, \quad A^{-1} = \begin{bmatrix} -1 & \sqrt{2} \\ \sqrt{2} & -1 \end{bmatrix}.$$

The matrix A is copositive because all of its entries are nonnegative. However, its inverse A^{-1} fails to be copositive.

Similar examples can be constructed in higher dimensions. In the above example, one sees that each column of A^{-1} contains at least one positive entry. This is not fortuitous, since such a behavior of A^{-1} can be predicted by a general result due to Valiaho [100, Theorem 3.4].

Proposition 7.7. *If $A \in \mathbb{S}_n$ is nonsingular and copositive, then each column of A^{-1} contains a positive entry.*

How likely is it to have A and A^{-1} copositive at the same time? An answer to the "strict" version of this question is given by the next theorem of Han and Mangasarian [51, Section 3].

Theorem 7.8. *Let $A \in \mathbb{S}_n$ be nonsingular. Then, the following statements are equivalent:*

(a) A and A^{-1} are strictly copositive.

(b) A is strictly copositive and A^{-1} is copositive.

(c) A is copositive and A^{-1} is strictly copositive.

(d) A is positive definite.

From a practical point of view, it is perhaps better to reformulate Theorem 7.8 in a negative way. Testing whether a given matrix $A \in \mathbb{S}_n$ is copositive is known to be coNP-complete, *i.e.*, testing whether A does not belong to $\mathcal{C}_n$ is NP-complete (*cf.* [72]). There are no polynomial time algorithms for checking copositivity, unless P=coNP. Testing whether $A \in \mathbb{S}_n$ is positive semidefinite can be answered, for example, by calculating the smallest eigenvalue of A (realm of numerical linear algebra); the same approach for copositivity by using $\mu(A)$ is a completely different story. So, if a nonsingular $A \in \mathbb{S}_n$ is known not to be positive definite, what can be said about its copositivity or that of A^{-1}? What Theorem 7.8 says is that:

$$A \in \mathbb{S}_n \text{ nonsingular and not positive definite} \quad \Longrightarrow \quad A \text{ or } A^{-1} \text{ is not strictly copositive.}$$

On the other hand, we mention that strictness is an essential requirement in the formulation of Theorem 7.8. Indeed, the copositivity of both A and A^{-1} does not guarantee the positive definiteness of A. The next example illustrates this point.

Example 7.9. Both matrices

$$A = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}, \quad A^{-1} = \begin{bmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix}$$

are copositive, but neither one is positive semidefinite.

As an alternative to the Han-Mangasarian approach, the question concerning the copositivity of both A and A^{-1} can be handled with the help of the next lemma established by Jacobson [65].

Lemma 7.10. *For a nonsingular $A \in \mathbb{S}_n$, the following statements are equivalent:*

(a) $\{x \in \mathbb{R}^n : x^T A x \geq 0\} \subset \{x \in \mathbb{R}^n : x^T A^{-1} x \geq 0\}$.

(b) There is a scalar $r \geq 0$ such that $A - rA^3$ is positive semidefinite.

Yes, A^3 stands for A to the power 3. Is not it weird such a result? Anyway, as a direct by-product of Jacobson's lemma, one obtains:

Corollary 7.11. *Let $A \in \mathbb{S}_n$ be nonsingular and copositive. Assume any of the following equivalent conditions:*

(a) The half-line $A - \mathbb{R}_+ A^3$ intersects the cone $\mathcal{P}_n$.

(b) There is a scalar $r \geq 0$ such that $\lambda_i(A) - r\,[\lambda_i(A)]^3 \geq 0$ for all $i \in \{1, \ldots, n\}$.

Then, also A^{-1} is copositive.

We strongly suspect that the copositivity of A^{-1} can be guaranteed under much weaker assumptions. As said before on a couple of occasions, usual eigenvalues are not sharp tools for dealing with copositivity issues.

7.5 Copositivity of a convex combination of quadratic forms

Yuan established in [103] a necessary and sufficient condition for a pair of symmetric matrices to admit a convex combination which is positive semidefinite.

Proposition 7.12. *Let $A, B \in \mathbb{S}_n$. Then, the following statements are equivalent:*

(a) There exists $t \in [0, 1]$ such that $(1-t)A + tB$ is positive semidefinite.

(b) $\max\{x^T A x,\, x^T B x\} \geq 0$ *for all $x \in \mathbb{R}^n_+$.*

When does a pair of symmetric matrices admit a convex combination which is copositive? Answering this question is not a trivial matter. The answer provided by Crouzeix *et al.* [30, Theorem 4.1] reads as follows.

Proposition 7.13. *Let $A, B \in \mathbb{S}_n$. Then, the following statements are equivalent:*

(a) There exists $t \in [0, 1]$ such that $(1-t)A + tB$ is copositive.

(b) $\max\{u^T A u + v^T A v,\, u^T B u + v^T B v\} \geq 0$ *for all $u, v \in \mathbb{R}^n_+$.*

Note that the condition (b) in Proposition 7.13 can be writen also in the "max-linear" form

$$\max\{\langle A, X\rangle, \langle B, X\rangle\} \geq 0 \quad \text{for all } X \in \mathcal{G}_n^{[2]},$$

where

$$\begin{aligned} \mathcal{G}_n^{[2]} &= \{X \in \mathcal{G}_n : \text{CP-rank}(X) \leq 2\} \\ &= \{uu^T + vv^T : u, v \in \mathbb{R}_+^n\}. \end{aligned}$$

So, this is a situation in which the CP-rank of a completely copositive matrix must be taken into account.

7.6 Copositivity, convexity, and Minty monotonicity

A symmetric matrix is positive semidefinite if and only if the associated quadratic form is a convex function. Is it possible to characterize the copositivity of $A \in \mathbb{S}_n$ by means of the convexity of q_A on a certain convex subset C of $\mathbb{R}^n$? Although this idea is natural, it turns out that such a way of handling copositivity leads to nowhere. First of all,

$$\begin{aligned} q_A \text{ is convex on } \mathbb{R}_+^n \quad &\iff \quad q_A \text{ is convex on the whole } \mathbb{R}^n \\ &\iff \quad A \text{ is positive semidefinite.} \end{aligned}$$

So, one must try with a set C that is smaller than the nonnegative orthant. What about the unit simplex? Once again, one misses the target:

$$q_A \text{ is convex on } \Lambda_n \quad \iff \quad x^T Ax \geq 0 \ \text{ whenever } \ x_1 + \ldots + x_n = 0.$$

All attempts in finding the right C will fail because such a convex set simply does not exist. The explanation of this fact is given below.

Proposition 7.14. *Let $A \in \mathbb{S}_n$ and C be a nonempty convex set in $\mathbb{R}^n$. The convexity of q_A on C is equivalent to the copositivity of A relative to the linear subspace $L_C = \mathbb{R}_+(C - C)$.*

Proof. That L_C is a linear subspace is clear. Note that q_A is convex on C if and only if, for any pair u, v of points in C, the second degree polynomial $t \in [0, 1] \mapsto q_A(u + t(v - u))$ is convex. This is yet equivalent to saying that

$$(v - u)^T A(v - u) \geq 0 \quad \text{for all } u, v \in C.$$

A simple homogeneity argument completes the proof. □

It is worthwhile to mention that copositivity of A on L_C is simply positive semidefiniteness of an associated matrix (namely of the matrix $G^T AG$, where the columns of G form a basis for L_C).

Is there a link between copositivity of A and some vague sort of convexity of q_A? This time the answer is yes, but the obtained result has a limited interest. Anyway, here is what one gets:

Proposition 7.15. *For $A \in \mathbb{S}_n$, the following statements are equivalent:*

(a) A is copositive.

(b) q_A satisfies the Jensen inequality

$$q_A((1-t)u+tv) \leq (1-t)q_A(u)+tq_A(v)$$

for all $t \in]0,1[$ and all $u, v \in \mathbb{R}^n$ such that $v-u \in \mathbb{R}^n_+$.

(c) For all $u \in \mathbb{R}^n$ and all $d \in \mathbb{R}^n_+$, the function q_A is convex on the half-line $u+\mathbb{R}_+d$.

An alternative characterization of positive semidefiniteness is Minty monotonicity of the gradient map of the associated quadratic form. Recall that a vector function $\Phi : \mathbb{R}^n \to \mathbb{R}^n$ is called Minty monotone if

$$[\Phi(v)-\Phi(u)]^T(v-u) \geq 0 \quad \text{for all } u, v \in \mathbb{R}^n.$$

Characterizing copositivity in terms of a Minty type monotonicity concept is also possible. However, as happens with Proposition 7.15, the obtained characterization is not very promising.

Proposition 7.16. *For $A \in \mathbb{S}_n$, the following statements are equivalent:*

(a) A is copositive.

(b) $[\nabla q_A(v)-\nabla q_A(u)]^T(v-u) \geq 0$ for all $u, v \in \mathbb{R}^n$ such that $v-u \in \mathbb{R}^n_+$.

Propositions 7.15 and 7.16 are both easy to prove. We mention them only because they provide a different angle for visualizing copositivity.

7.7 Understanding copositivity via nonsmooth analysis

Projecting onto a closed convex cone is a typical example of an operation that lacks differentiability. For instance, projecting $x \in \mathbb{R}^n$ onto the nonnegative orthant $\mathbb{R}^n_+$ produces the vector

$$x^+ = (x_1^+, \ldots, x_n^+)^T$$

whose components $x_i^+ = \max\{x_i, 0\}$ are clearly nondifferentiable. If one accepts working with nonsmooth functions, then a large avenue is open for characterizing copositivity in the most diverse and unexpected ways. A first result in this line concerns the use of the function

$$x \in \mathbb{R}^n \mapsto Q_{A,\kappa}(x) = x^TAx + \kappa \|x^+\|^2, \tag{67}$$

which can be seen as a "penalized" version of the quadratic form q_A. Note that $x \in \mathbb{R}^n \mapsto \|x^+\|^2$ is differentiable, but not twice differentiable.

Theorem 7.17. *For $A \in \mathbb{S}_n$, the following statements are equivalent:*

(a) A is strictly copositive.

(b) There exists a "penalty" parameter $\kappa \geq 0$ such that

$$x^TAx + \kappa \|x^+\|^2 > 0 \qquad \text{for all } x \in \mathbb{R}^n \backslash \{0\}. \tag{68}$$

Proof. Clearly $x^+ = 0$ whenever $x \in \mathbb{R}^n_-$. Hence, the relation (68) yields in particular

$$x^T Ax > 0 \qquad \text{for all } x \in \mathbb{R}^n_- \backslash \{0\},$$

which is just another way of expressing the strict copositivity of A. Conversely, let A be strictly copositive. Ab absurdo, suppose that (b) does not hold. Then, for any integer $k \geq 1$, there exists a nonzero vector $x^{(k)}$ in $\mathbb{R}^n$ such that

$$(x^{(k)})^T Ax^{(k)} + k \left\| (x^{(k)})^+ \right\|^2 \leq 0.$$

Hence, the normalized vector $u^{(k)} = x^{(k)} / \left\| x^{(k)} \right\|$ satisfies

$$\frac{(u^{(k)})^T Au^{(k)}}{k} + \left\| (u^{(k)})^+ \right\|^2 \leq 0 \quad \text{for all } k \geq 1. \tag{69}$$

Extracting a subsequence if necessary, we may suppose that $\{u^{(k)}\}_{k\geq 1}$ converges to some unit vector $u \in \mathbb{R}^n$. Passing to the limit in (69), one gets $u^+ = 0$, that is to say, u belongs to $\mathbb{R}^n_-$. We now use the strict copositivity of A in order to write $u^T Au > 0$. In turn, this inequality implies that $(u^{(k)})^T Au^{(k)} > 0$ for all k large enough, contradicting the relation (69). □

Remark 7.18. The most striking feature of the inequality (68) is that the argument x is not forced to lie on the cone $\mathbb{R}^n_+$ (or, what is equivalent, on the cone $\mathbb{R}^n_-$). The conic restriction has been removed or, more precisely, it has been incorporated in the penalty term $\|x^+\|^2$. By the way, Theorem 7.17 could have been written by using instead the penalty term $\|x^-\|^2$, where $x^- = (x_1^-, \ldots, x_n^-)^T$ is the vector whose i-th component is given by $x_i^- = \max\{-x_i, 0\}$. As everyone working in optimization, we stick to the old habit of giving the preference to x^+ over x^-.

Theorem 7.17 admits also a nonstrict version, but its formulation is a bit more elaborate. For convenience, we introduce first a slight variant of the concept of copositivity.

Definition 7.19. *A matrix $A \in \mathbb{S}_n$ is supra-copositive if there is a real $\kappa \geq 0$ such that*

$$x^T Ax + \kappa \|x^+\|^2 \geq 0 \qquad \textit{for all } x \in \mathbb{R}^n. \tag{70}$$

The infimum of all $\kappa \geq 0$ satisfying (70) is denoted by $\kappa(A)$.

The link between copositivity and supra-copositivity is explained in the next theorem, see also Figure 1.

Theorem 7.20. *For $A \in \mathbb{S}_n$, the following statements hold true:*

(a) If A is supra-copositive, then A is copositive.

(b) If A is copositive, then A can be expressed as limit of supra-copositive matrices, say $A = \lim_{r\to\infty} A^{(r)}$. The limit itself does need to be supra-copositive. Failure of supra-copositivity in the limit is reflected by the fact that $\{\kappa(A^{(r)})\}_{r\geq 1}$ is an unbounded sequence.

Proof. Part (a) is proven as in Theorem 7.17. In order to prove (b), we introduce the set

$$\mathcal{E}_n = \{A \in \mathbb{S}_n : A \text{ is supra-copositive}\}.$$

One can easily check that $\mathcal{E}_n$ is a convex cone. Thanks to Theorem 7.17, any strictly copositive matrix is supra-copositive. So far, we have shown that

$$\text{int}(\mathcal{C}_n) \subset \mathcal{E}_n \subset \mathcal{C}_n.$$

This, of course, implies that $\mathcal{C}_n$ is the closure of $\mathcal{E}_n$. Finally, suppose that $A \in \mathcal{C}_n \backslash \mathcal{E}_n$ and write $A = \lim_{r\to\infty} A^{(r)}$ as limit of supra-copositive matrices. Suppose, on the contrary, that $\{\kappa(A^{(r)})\}_{r\geq 1}$ is bounded. Taking a subsequence if necessary, one may assume that $\bar{\kappa} = \lim_{r\to\infty} \kappa(A^{(r)})$ exists. Pick any $\varepsilon > 0$. By fixing $x \in \mathbb{R}^n$ and passing to the limit in

$$x^T A^{(r)} x + \left(\kappa(A^{(r)}) + \varepsilon\right) \|x^+\|^2 \geq 0,$$

one arrives at a contradiction, namely, that A is supra-copositive (with $\kappa(A) \leq \bar{\kappa} + \varepsilon$). □

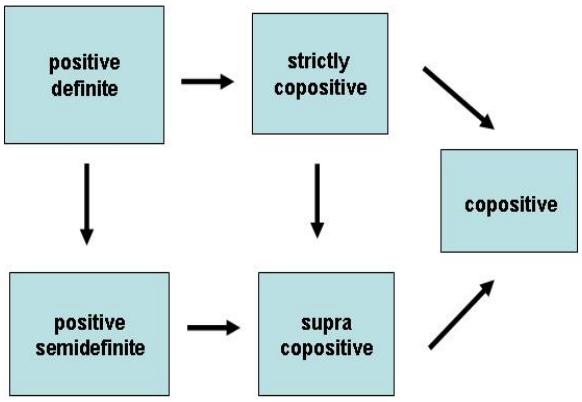

Figure 1: Manifolds paths leading to copositivity. All implications are irreversible.

Although less interesting than (67), another option is considering the parameter-free nonsmooth function

$$x \in \mathbb{R}^n \mapsto f_A(x) = (x^+)^T A x^+. \tag{71}$$

Such a pseudo-quadratic form corresponds to the composition of the quadratic form q_A and the projection operator $x \mapsto x^+$.

Proposition 7.21. *$A \in \mathbb{S}_n$ is copositive if and only if $(x^+)^T A x^+ \geq 0$ for all $x \in \mathbb{R}^n$.*

The above proposition is trivial. It is not clear to us whether such a characterization of copositivity has a potential use or not. Anyway, it is worth mentioning that (71) is positively homogeneous of degree two, and therefore the copositivity of A amounts to the nonnegativity of the coefficient

$$\xi(A) = \inf_{\|x\|=1} (x^+)^T A x^+. \tag{72}$$

The cost function in (72) is nonsmooth, but the constraint $x \geq 0$ does not show up. The above minimization problem is structurally different from the old minimization problem (1). In particular, the criticality conditions for (72) lead to a multivalued spectral theory that can be developed as an alternative to the Pareto spectral analysis.

7.8 Copositivity and Legendre-Fenchel conjugation

Since our survey has an optimization or variational flavor, let us see in this paragraph what Legendre-Fenchel conjugation could provide as additional information on copositivity. Recall that the (Legendre-Fenchel) conjugate of an extended-real-valued function φ on $\mathbb{R}^n$ is another extended-real-valued function on $\mathbb{R}^n$, denoted by φ^* and given by

$$\varphi^*(y) = \sup_{x \in \mathbb{R}^n} \{y^T x - \varphi(x)\}.$$

A clever application of the theory of conjugate functions leads to the next result, which is a rather unorthodox characterization of copositivity.

Theorem 7.22. *Let $A \in \mathbb{S}_n$. Consider any parameter κ positive and larger than $\lambda_{\max}(A)$. Then, A is copositive if and only if*

$$y^T(\kappa I_n - A)^{-1} y \geq \frac{1}{\kappa} \|y^+\|^2 \quad \textit{for all } y \in \mathbb{R}^n. \tag{73}$$

Proof. That $A \in \mathbb{S}_n$ is copositive can be expressed in the "unconstrained" form

$$-(1/2)\, x^T A x \leq \Psi_{\mathbb{R}^n_+}(x) \quad \text{for all } x \in \mathbb{R}^n, \tag{74}$$

where Ψ_Ω stands for the indicator function of a given set Ω in $\mathbb{R}^n$, *i.e.*,

$$\Psi_\Omega(x) = \begin{cases} 0 & \text{if} \quad x \in \Omega \\ +\infty & \text{if} \quad x \notin \Omega. \end{cases}$$

The factor $1/2$ in front of the quadratic form has been introduced only for computational convenience. By adding the term $(\kappa/2)\,\|x\|^2$ on each side of (74), one gets an equivalent inequality

$$\overbrace{(1/2)\, x^T(\kappa I_n - A)x}^{g(x)} \;\leq\; \overbrace{(\kappa/2)\|x\|^2 + \Psi_{\mathbb{R}^n_+}(x)}^{h(x)} \quad \text{for all } x \in \mathbb{R}^n$$

that has the merit of comparing two convex functions. The way the parameter κ has been chosen ensures the positive definiteness of the matrix $\kappa I_n - A$. Since the Legendre-Fenchel conjugation of convex functions reverse the order of inequalities, the copositivity of A is yet equivalent to

$$\overbrace{(1/2)\, y^T(\kappa I_n - A)^{-1} y}^{g^*(y)} \;\geq\; \overbrace{(1/2\kappa)\|y^+\|^2}^{h^*(y)} \quad \text{for all } y \in \mathbb{R}^n.$$

This completes the proof of the theorem. □

The result of Theorem 7.22 resembles that of Theorem 7.17. This time, however, the leading role is played by the resolvent map $\kappa \mapsto (\kappa I_n - A)^{-1}$, and not by A itself. For this reason, we baptize (73) as the resolvent characterization of copositivity. A direct by-product of Theorem 7.22 is this: if A is copositive, then $(\kappa I_n - A)^{-1}$ is strictly copositive for all $\kappa > \lambda_{\max}(A)$. Simple examples show that the converse is not true.

8 By way of conclusion

There are still many things one could say about copositity, but at some moment we must put an end to this survey. Our last lines are devoted to two important items, but we shall not treat them in extenso. Some brief remarks and suggestions of further reading will be enough.

8.1 Testing copositivity in high dimensions

The copositivity detection methods mentioned in Sections 3 and 4 are well suited for matrices of moderate order. Copositivity tests intended for matrices of large order have been proposed in [15, 22, 31, 56, 89]. We briefly recall the approach of Parrilo [89]. It consists in approximating $\mathcal{C}_n$ to any given accuracy by another convex cone $\mathcal{C}_n^{(r)}$ that depends on a nonnegative integer r. By definition, the approximating cone $\mathcal{C}_n^{(r)}$ contains $A \in \mathbb{S}_n$ if and only if the multivariate polynomial

$$u \in \mathbb{R}^n \mapsto P_{A,r}(u) = \left(\sum_{i,j=1}^{n} a_{i,j} u_i^2 u_j^2 \right) \left(\sum_{i=1}^{n} u_i^2 \right)^r \tag{75}$$

admits a sum-of-squares decomposition.

Notice that the first factor in the product (75) corresponds to the quartic multivariate polynomial introduced in Corollary 5.3. Hence, $\mathcal{C}_n^{(0)} \subset \mathcal{C}_n$. Better inner approximations of $\mathcal{C}_n$ are obtained by successively increasing the parameter r:

$$\mathcal{C}_n^{(0)} \subset \mathcal{C}_n^{(1)} \subset \mathcal{C}_n^{(2)} \subset \ldots \subset \mathcal{C}_n.$$

The big merit of Parrilo's approach is that membership in a given $\mathcal{C}_n^{(r)}$ can be tested by solving a certain system of Linear Matrix Inequalities (LMI), so one is back in the better known realm of semidefinite programming.

8.2 Copositivity as tool for optimization modeling

Copositivity helps in the reformulation of difficult nonconvex quadratic programs. A recent line of research has shown that several NP-hard optimization problems can be expressed as linear programs over $\mathcal{C}_n$. Burer [23] provides a long (and presumably complete) list of problems known to have a linear copositive programming representation.

Sometimes the leading role is played by the dual cone $\mathcal{G}_n$, and not by the original cone $\mathcal{C}_n$. For instance, Burer [23] models any nonconvex quadratic program having a mix of binary and

continuous variables as a linear program over $\mathcal{G}_n$. The general-form problem considered there is:

$$\begin{array}{c} \text{Minimize} \quad x^T Q x + 2c^T x \\ a_i^T x = b_i \text{ for } i \in I \\ x \geqslant 0 \\ x_j \in \{0,1\} \text{ for } j \in J \end{array} \tag{76}$$

with $I = \{1, ..., m\}$ indexing linear equality constraints, and $J \subset \{1, ..., n\}$ indexing the components of x that are required to be binary.

Under mild assumptions (*cf.* [23, Theorem 2.6]), the above problem is shown to be equivalent to the problem below (in the variables x and X):

$$\begin{array}{c} \text{Minimize} \quad \langle Q, X \rangle + 2c^T x \\ a_i^T x = b_i \text{ for } i \in I \\ \left\langle a_i a_i^T, X \right\rangle = b_i^2 \text{ for } i \in I \\ x_j = X_{jj} \text{ for all } j \in J \\ \left[\begin{array}{cc} 1 & x^T \\ x & X \end{array} \right] \in \mathcal{G}_{n+1}. \end{array} \tag{77}$$

The equivalence between (76) and (77) must be understood in the following sense: both problems have same the optimal value, and if $(\overline{x}, \overline{X})$ is a solution to (77), then $\overline{x}$ lies in the convex hull of the solution set to (76). Hence, a broad class of NP-hard problems can be transformed into a specific class of well-structured convex minimization problems. However, the difficulty of (76) is transferred in the last constraint of (77), namely the completely positive constraint. Unfortunately, there is no known self-concordant barrier function naturally associated with $\mathcal{G}_n$ or $\mathcal{C}_n$, as is the case with $\mathcal{P}_n$.

Remark 8.1. As rightly pointed out by one of the referees, the approximations $\mathcal{C}_n^{(r)}$ of $\mathcal{C}_n$ and their dual cones $\mathcal{G}_n^{(r)}$ can be used to achieve tractable approximations of (77).

There are many other interesting references concerning the role of copositivity in the modeling and analysis of optimization problems. We mention [2, 18, 19, 32, 33, 95], but this list is by no means exhaustive.

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