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A Square Departure From Symmetry in Matrix Cones

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Abstract
Conic optimization problems are usually understood to be problems over some cone of symmetric matrices like the semidefinite or the copositive matrix cone. In this note, we investigate the changes that have to be made when moving from symmetric to nonsymmetric matrices. We introduce the proper definitions and study the dual of a cone of nonsymmetric matrices. Next, we attempt to generalize the well known concept of cp-rank to nonsymmetric matrices. Finally, we derive some new results on symmetric and nonsymmetric copositive-plus matrices.

Keywords Conic optimization · Nonsymmetric copositive and completely positive matrices · Nonsymmetric cp-rank · Copositive-plus matrices

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1 Introduction

The cone of symmetric copositive matrices and its dual cone of symmetric completely positive matrices have proved extremely useful in combinatorial optimization and nonconvex quadratic programming. Tamás Terlaky was one of the pioneers of this field: in [20], he and his co-authors studied nonconvex quadratic problems and proposed a relaxation using copositive matrices which strengthened the well known semidefinite Shor relaxation. Two years later, Terlaky was the co-author of another paper [4] which for the first time established that a combinatorial problem (namely, the maximum clique problem) can equivalently be rewritten as a linear optimization problem over the cone of copositive matrices. This result was based on earlier results by Motzkin and Straus [19] and by Bomze [3], with a regularization ensuring full one-to-one correspondence of local solutions to a continuous quadratic problem on one

This paper is dedicated to Tamás Terlaky on the occasion of his 70th birthday.

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side, and maximal cliques on the other side, a maximum clique being encoded uniquely by a global solution to the quadratic problem (the formulation in [3] avoids spurious solutions which could occur with the formulation in [19]; see also [17] for a more recent account, in particular Fig.1 on p.1166 there for a counterexample). Returning to Terlaky's contributions, the paper [4] also introduced the notion "copositive optimization" and introduced a field which has been highly active ever since. See [11] for a recent survey.

Copositive optimization, like semidefinite optimization, is a subclass of conic optimization, where one generally aims to minimize a linear or nonlinear function subject to the constraint that the matrix variable is in some closed convex cone $\mathcal{K}$ of symmetric matrices. Its dual problem involves the dual cone $\mathcal{K}^*$. In case $\mathcal{K}$ is the copositive cone, its dual is the cone of completely positive matrices. Both cones have been studied intensively not only in the optimization community, but also in the linear algebra community. For a good overview on those more structural properties of these cones, we refer to [21].

A common feature is that so far, researchers have only studied symmetric copositive and completely positive matrices. To the best of our knowledge, nobody has attempted to generalize known results to the nonsymmetric case. In this note, we make a first attempt in this direction: we investigate the changes that are necessary when moving from symmetric to nonsymmetric matrices. We introduce the notion of nonsymmetric copositive and completely positive matrices and study the relations between both situations. Note that nonsymmetric matrices play a prominent role in linear complementarity problems, in particular when applied to quadratic optimization, cf. [9].

Next, we are interested in the so called cp-rank of a symmetric completely positive matrix which in a sense describes the size of a minimal factorization of such a matrix (for a precise definition, see below). We attempt to generalize the cp-rank to the nonsymmetric case and propose three possible variants.

Finally, we study a subset of the cone of copositive matrices, namely so-called copositive-plus matrices. These, again, play an important role for linear complementarity problems, see [9]. We revisit this class and show several new results both for the symmetric and for the nonsymmetric case.

Notation Denote by $\mathbb{N}$ the set of positive integers. For $\alpha \in \mathbb{R}$, we put $(\alpha)_+ := \max\{\alpha, 0\}$. We write

$$\Delta^n := \left\{\mathbf{x} \in \mathbb{R}^n_+ : \mathbf{e}^\top \mathbf{x} = 1\right\} \quad \text{and} \quad \mathbf{e} = [1, \dots, 1]^\top \in \mathbb{R}^n.$$

Denote by $\sigma(\mathbf{x}) := \{i : x_i > 0\}$ the support of an $\mathbf{x} \in \Delta^n$ and by $\mathsf{I}_n := \mathrm{Diag}(\mathbf{e})$ the $n \times n$-identity matrix, with columns $\mathbf{e}_i$ $(i = 1, \dots, n)$. The inner product on $\mathbb{R}^{n\times n}$ is the Frobenius product: $\langle \mathsf{A}, \mathsf{B}\rangle := \mathrm{tr}(\mathsf{A}^\top \mathsf{B})$. Moreover,

$$\mathcal{S}_n := \{\mathsf{S} \in \mathbb{R}^{n\times n} : \mathsf{S}^\top = \mathsf{S}\} \quad \text{denotes the space of symmetric matrices and}$$
$$\mathcal{W}_n := \{\mathsf{W} \in \mathbb{R}^{n\times n} : \mathsf{W}^\top = -\mathsf{W}\} \quad \text{the space of skew-symmetric matrices.}$$

The following relations between $\mathcal{S}_n$ and $\mathcal{W}_n$ should be well known:

Lemma 1.1 *We have* $\mathcal{W}_n = \mathcal{S}_n^\perp$ *with* $\dim \mathcal{S}_n = \frac{1}{2}n(n+1)$ *and* $\dim \mathcal{W}_n = \frac{1}{2}(n-1)n$. *Hence* $\mathbb{R}^{n\times n} = \mathcal{S}_n \oplus \mathcal{W}_n$, *and the corresponding unique decomposition of* $\mathsf{X} \in \mathbb{R}^{n\times n}$ *is* $\mathsf{X} = \frac{1}{2}(\mathsf{X} + \mathsf{X}^\top) + \frac{1}{2}(\mathsf{X} - \mathsf{X}^\top)$.

Proof Let $\mathsf{S} \in \mathcal{S}_n$ and $\mathsf{W} \in \mathcal{W}_n$. Then

$$\begin{aligned}\langle \mathsf{W}, \mathsf{S}\rangle &= \mathrm{tr}(\mathsf{W}^\top \mathsf{S}) = -\mathrm{tr}(\mathsf{W}\mathsf{S}) = -\mathrm{tr}(\mathsf{S}^\top \mathsf{W}^\top) \\ &= -\mathrm{tr}(\mathsf{S}\mathsf{W}^\top) = -\mathrm{tr}(\mathsf{W}^\top \mathsf{S}) = -\langle \mathsf{W}, \mathsf{S}\rangle,\end{aligned}$$

so $\langle \mathsf{S}, \mathsf{W} \rangle = 0$. The other assertions are trivial. □

We will also study the following subcones of $\mathcal{S}_n$:

$$\mathcal{N}_n := \mathcal{S}_n \cap \mathbb{R}_+^{n\times n} = \{\mathsf{N} \in \mathcal{S}_n : N_{ij} \geq 0 \text{ for all } i, j\}, \quad \text{the cone of entrywise nonnegative matrices,}$$

$$\mathcal{S}_n^+ := \{\mathsf{S} \in \mathcal{S}_n : \mathbf{x}^\top \mathsf{S}\mathbf{x} \geq 0 \text{ for all } \mathbf{x} \in \mathbb{R}^n\}, \quad \text{the positive-semidefinite cone,}$$

$$\mathcal{COP}_n := \{\mathsf{S} \in \mathcal{S}_n : \mathbf{x}^\top \mathsf{S}\mathbf{x} \geq 0 \text{ for all } \mathbf{x} \in \mathbb{R}_+^n\}, \quad \text{the copositive cone,}$$

$$\mathcal{CP}_n := \{\mathsf{S} \in \mathcal{S}_n : \mathsf{S} = \mathsf{F}^\top \mathsf{F} \text{ for some } \mathsf{F} \in \mathbb{R}_+^{p\times n}\}, \quad \text{the completely positive cone.}$$

In the definition of $\mathcal{CP}_n$, $p \in \mathbb{N}$ is an upper bound for the so-called cp-rank of a matrix in $\mathcal{CP}_n$, see [22, 23]. We may choose $p \leq p_n := \binom{n+1}{2} - 4$, where p_n is an asymptotically tight upper bound, cf. [6].

We will often omit the index n for notational convenience. Also, we will call any matrix $\mathsf{Q} \in \mathcal{COP} \setminus (\mathcal{S}^+ + \mathcal{N})$ *exceptional.*

2 Duality Results

Let $\mathcal{K} \subseteq \mathcal{S} \subseteq \mathbb{R}^{n\times n}$, and denote by $\mathcal{K}^*$ the dual of $\mathcal{K}$ when $\mathcal{S}$ is considered as the underlying space, i.e.,

$$\mathcal{K}^* := \{\mathsf{X} \in \mathcal{S} : \langle \mathsf{X}, \mathsf{K} \rangle \geq 0 \text{ for all } \mathsf{K} \in \mathcal{K}\}.$$

It is well known that

$$\mathcal{N}^* = \mathcal{N}, \quad (\mathcal{S}^+)^* = \mathcal{S}^+, \quad \mathcal{COP}^* = \mathcal{CP}, \quad \mathcal{CP}^* = \mathcal{COP}.$$

Note that this definition only makes sense for subcones of $\mathcal{S}$. However, for $\mathcal{K} \subseteq \mathbb{R}^{n\times n}$ we define $\mathcal{K}^{\overline{*}}$ to be the dual of $\mathcal{K}$ when $\mathbb{R}^{n\times n}$ is considered as the underlying space, i.e.,

$$\mathcal{K}^{\overline{*}} := \{\mathsf{X} \in \mathbb{R}^{n\times n} : \langle \mathsf{X}, \mathsf{K} \rangle \geq 0 \text{ for all } \mathsf{K} \in \mathcal{K}\}.$$

It is easy to see that the dual of a linear subspace is its orthogonal complement, and therefore

$$\mathcal{S}^{\overline{*}} = \mathcal{W} \quad \text{and} \quad \mathcal{W}^{\overline{*}} = \mathcal{S}. \tag{1}$$

We are interested in the relation between the duals $\mathcal{K}^{\overline{*}}$ and $\mathcal{K}^*$ of a cone $\mathcal{K} \subseteq \mathcal{S}$ of symmetric matrices. This is clarified in the next theorem.

Theorem 2.1 *For $\mathcal{K} \subseteq \mathcal{S} \subseteq \mathbb{R}^{n\times n}$, we have $\mathcal{K}^{\overline{*}} = \mathcal{K}^* + \mathcal{W}$.*

Proof Let $\mathsf{X} \in \mathcal{K}^{\overline{*}}$. Writing $\mathsf{X} = \mathsf{S} + \mathsf{W}$ with $\mathsf{S} \in \mathcal{S}$ and $\mathsf{W} \in \mathcal{W}$, we get using Lemma 1.1 that for all $\mathsf{K} \in \mathcal{K}$,

$$0 \leq \langle \mathsf{X}, \mathsf{K} \rangle = \langle \mathsf{S}, \mathsf{K} \rangle + \langle \mathsf{W}, \mathsf{K} \rangle = \langle \mathsf{S}, \mathsf{K} \rangle,$$

so $\mathsf{S} \in \mathcal{K}^*$ and one inclusion is proved. To show the reverse inclusion, take $\mathsf{S} \in \mathcal{K}^*$ and $\mathsf{W} \in \mathcal{W}$. Then $\mathsf{X} := \mathsf{S} + \mathsf{W}$ is in $\mathcal{K}^{\overline{*}}$, since, again by Lemma 1.1, we have that $\langle \mathsf{X}, \mathsf{K} \rangle = \langle \mathsf{S}, \mathsf{K} \rangle + \langle \mathsf{W}, \mathsf{K} \rangle = \langle \mathsf{S}, \mathsf{K} \rangle \geq 0$ for all $\mathsf{K} \in \mathcal{K}$. □

For a matrix $\mathsf{X} \in \mathbb{R}^{n\times n}$, we write

$$\overline{\mathsf{X}} := \tfrac{1}{2}(\mathsf{X} + \mathsf{X}^\top) \in \mathcal{S}_n.$$

For $\mathcal{K} \subseteq \mathcal{S} \subset \mathbb{R}^{n\times n}$, we define its desymmetrized version as follows:

$$\overline{\mathcal{K}} := \{\mathsf{X} \in \mathbb{R}^{n\times n} : \overline{\mathsf{X}} \in \mathcal{K}\}.$$

This definition includes the set $\overline{\mathcal{S}^+}$ of nonsymmetric positive-semidefinite matrices and the set $\overline{\mathcal{COP}}$ of nonsymmetric copositive matrices, because both definitions are based on signs of quadratic forms where symmetry does not play a role. For $\mathcal{K} \in \{\mathcal{N}, \mathcal{CP}\}$ the situation is different, as shown by the following lemma.

Lemma 2.2 *For $\mathcal{K} \subseteq \mathcal{S} \subset \mathbb{R}^{n\times n}$, we have:*

(a) $\overline{\mathcal{K}} = \mathcal{K} + \mathcal{W}$,
(b) *If $\mathcal{K}$ is closed and $n > 1$, then $\overline{\mathcal{K}}$ is a closed, non-pointed cone.*

Proof (a) Take $\mathsf{X} \in \overline{\mathcal{K}}$ and decompose $\mathsf{X} = \overline{\mathsf{X}} + \frac{1}{2}(\mathsf{X} - \mathsf{X}^\top) \in \mathcal{K} + \mathcal{W}$. This proves one inclusion. To see the reverse one, take $\mathsf{X} = \mathsf{K} + \mathsf{W} \in \mathcal{K} + \mathcal{W}$. Then $\mathsf{X} + \mathsf{X}^\top = 2\mathsf{K} \in \mathcal{K}$, so $\mathsf{X} \in \overline{\mathcal{K}}$.
(b) If $\mathsf{O} \in \mathcal{K}$, then obviously $\mathsf{O} \in \overline{\mathcal{K}}$, so $\overline{\mathcal{K}}$ is closed, and not pointed since $\{\mathsf{O}\} \neq \mathcal{W} \subseteq \overline{\mathcal{K}} \cap (-\overline{\mathcal{K}})$ by virtue of (a) and $\mathsf{O} \in \mathcal{K}$. □

Remark 2.3 The above situation is a special case of the following constellation: consider a self-adjoint, surjective linear map $\mathcal{L} : \mathbb{E} \to \mathcal{S}$, where $\mathbb{E}$ is a Euclidean space and $\mathcal{S}$ is a linear subspace of $\mathbb{E}$. For any closed cone $\mathcal{K} \subseteq \mathcal{S}$, define the set $\overline{\mathcal{K}} := \mathcal{L}^{-1}(\mathcal{K})$, which is again a closed cone. Now, if $\mathcal{W} = \mathcal{S}^\perp$, then most of the above duality results carry over by the same arguments as for the special case $\mathbb{E} = \mathbb{R}^{n\times n}$, $\mathcal{L}(\mathsf{X}) = \overline{\mathsf{X}}$ and the Frobenius inner product.

It is well known that a cone $\mathcal{C} \subset \mathbb{R}^{n\times n}$ is pointed if and only if its dual $\mathcal{C}^{\overline{*}}$ is full dimensional. More precisely, it is not difficult to show that codim $\mathcal{C}^{\overline{*}} = \dim(\mathcal{C} \cap (-\mathcal{C}))$. In view of this, the next result is unsurprising:

Theorem 2.4 *For $\mathcal{K} \subseteq \mathcal{S} \subset \mathbb{R}^{n\times n}$, we have $\overline{\mathcal{K}}^{\overline{*}} = \mathcal{K}^*$ and $\mathcal{K}^{\overline{*}} = \overline{\mathcal{K}^*}$.*

Proof By Lemma 2.2(a), Theorem 2.1 and (1), we have

$$\overline{\mathcal{K}}^{\overline{*}} = (\mathcal{K} + \mathcal{W})^{\overline{*}} = \mathcal{K}^{\overline{*}} \cap \mathcal{W}^{\overline{*}} = (\mathcal{K}^* + \mathcal{W}) \cap \mathcal{S} = \mathcal{K}^*.$$

The second assertion is a standard duality argument, but also comes easily from Theorem 2.1 and Lemma 2.2(a):

$$\mathcal{K}^{\overline{*}} = \mathcal{K}^* + \mathcal{W} = \overline{\mathcal{K}^*}.$$

Hence the result. □

As a consequence, we immediately get the following.

Corollary 2.5 *We have:*

(a) $\mathcal{N}^{\overline{*}} = \overline{\mathcal{N}}$ *and* $\overline{\mathcal{N}}^{\overline{*}} = \mathcal{N}$,
(b) $(\mathcal{S}^+)^{\overline{*}} = \overline{\mathcal{S}^+}$ *and* $\overline{\mathcal{S}^+}^{\overline{*}} = \mathcal{S}^+$,
(c) $\mathcal{CP}^{\overline{*}} = \overline{\mathcal{COP}}$ *and* $\overline{\mathcal{COP}}^{\overline{*}} = \mathcal{CP}$,
(d) $\mathcal{COP}^{\overline{*}} = \overline{\mathcal{CP}}$ *and* $\overline{\mathcal{CP}}^{\overline{*}} = \mathcal{COP}$.

Let us now look at *minimum distance projections* with respect to the norm $\|\mathsf{A}\| := \sqrt{\langle \mathsf{A}, \mathsf{A}\rangle}$ of a matrix $\mathsf{A} \in \mathbb{R}^{n\times n}$ onto a closed convex set $\mathcal{C} \subset \mathbb{R}^{n\times n}$. It is well known that this projection $\Pi_{\mathcal{C}}$ is given by the unique $\mathsf{Y} \in \mathcal{C}$ satisfying

$$\|\mathsf{X} - \mathsf{Y}\| \leq \|\mathsf{X} - \mathsf{Z}\| \quad \text{for all } \mathsf{Z} \in \mathcal{C}.$$

In other words,

$$\Pi_{\mathcal{C}}\mathsf{X} := \operatorname{argmin}\{\|\mathsf{X} - \mathsf{Z}\| : \mathsf{Z} \in \mathcal{C}\}.$$

It is well known that $\mathsf{Y} := \Pi_{\mathcal{C}}\mathsf{X}$ is characterized by the Stampacchia variational inequality

$$\langle \mathsf{X} - \mathsf{Y}, \mathsf{Z} - \mathsf{Y}\rangle \leq 0 \quad \text{for all } \mathsf{Z} \in \mathcal{C}. \tag{2}$$

Specializing $\mathcal{C}$ to closed convex cones $\mathcal{K} \subseteq \mathcal{S}$, we can characterize Y further:

Theorem 2.6 *Let $\mathcal{K} \subseteq \mathcal{S}_n$ be a closed convex cone, and let $\mathsf{X} \in \mathbb{R}^{n\times n}$ be an arbitrary square matrix. Then*

$$\mathsf{Y} := \Pi_{\mathcal{K}}\mathsf{X} = \bar{\mathsf{X}} + \mathsf{C} \tag{3}$$

for some $\mathsf{C} \in \mathcal{K}^*$ supporting $\mathcal{K}$ at Y, i.e.

$$\langle \mathsf{C}, \mathsf{Y}\rangle = 0 \leq \langle \mathsf{C}, \mathsf{Z}\rangle \quad \textit{for all } \mathsf{Z} \in \mathcal{K} \tag{4}$$

(by slight abuse of terminology, we use "supporting" also if $\mathsf{C} = \mathsf{O}$).

Conversely, if for some $\mathsf{C} \in \mathcal{K}^*$, we have $\mathsf{C} \perp \mathsf{Y} = \bar{\mathsf{X}} + \mathsf{C} \in \mathcal{K}$, then $\mathsf{Y} = \Pi_{\mathcal{K}}\mathsf{X}$.

Proof Consider (2) for a cone $\mathcal{K}$:

$$\langle \mathsf{X} - \mathsf{Y}, \mathsf{Z}\rangle \leq \langle \mathsf{X} - \mathsf{Y}, \mathsf{Y}\rangle \quad \text{for all } \mathsf{Z} \in \mathcal{K}.$$

From this, it easily follows that $\langle \mathsf{X} - \mathsf{Y}, \mathsf{Z}\rangle \leq 0$ for all $\mathsf{Z} \in \mathcal{K}$, and hence we get by Theorem 2.1 that

$$\mathsf{Y} - \mathsf{X} \in \overline{\mathcal{K}^*} = \mathcal{K}^* + \mathcal{W}_n.$$

So $\mathsf{Y} = \mathsf{X} + \mathsf{C} + \mathsf{W}$ with $\mathsf{C} \in \mathcal{K}^* \subseteq \mathcal{S}_n$ and $\mathsf{W}^\top = -\mathsf{W} \in \mathbb{R}^{n\times n}$. But $\mathsf{Y}^\top \in \mathcal{K} \subseteq \mathcal{S}_n$ by construction. We conclude that

$$2\mathsf{Y} = \mathsf{Y} + \mathsf{Y}^\top = 2\mathsf{C} + \mathsf{X} + \mathsf{X}^\top + \mathsf{O}$$

or $\mathsf{Y} = \bar{\mathsf{X}} + \mathsf{C}$. Defining $\widehat{\mathsf{X}} := \frac{1}{2}(\mathsf{X} - \mathsf{X}^\top) \in \mathcal{W}_n$ and using (2), we see that

$$\langle \widehat{\mathsf{X}} - \mathsf{C}, \mathsf{Z} - \bar{\mathsf{X}} - \mathsf{C}\rangle = \langle \mathsf{X} - \mathsf{Y}, \mathsf{Z} - \mathsf{Y}\rangle \leq 0 \quad \text{for all } \mathsf{Z} \in \mathcal{K}.$$

But since $\mathsf{Z} - \bar{\mathsf{X}} - \mathsf{C} \in \mathcal{S}_n$, Lemma 1.1 implies that

$$\langle \widehat{\mathsf{X}}, \mathsf{Z} - \bar{\mathsf{X}} - \mathsf{C}\rangle = 0.$$

So we conclude that

$$\langle \mathsf{C}, \mathsf{Z} - \mathsf{Y}\rangle \geq 0 \quad \text{for all } \mathsf{Z} \in \mathcal{K}. \tag{5}$$

In particular for $\mathsf{Z} = \mathsf{O} \in \mathcal{K}$ (since $\mathcal{K}$ is closed), we get

$$0 \leq \langle \mathsf{C}, \mathsf{Y}\rangle \leq 0,$$

where the left inequality follows from duality and the right one from (5). Hence $\mathsf{C} \perp \mathsf{Y}$ and therefore (4) is established. The converse follows because (4) is the same as (2) which implies $\mathsf{Y} = \Pi_{\mathcal{K}}\mathsf{X}$, as mentioned before for general closed convex $\mathcal{C}$. □

Another way of expressing (3) is $\Pi_{\mathcal{K}} \circ \Pi_{\mathcal{S}} = \Pi_{\mathcal{K}} = \Pi_{\mathcal{S}} \circ \Pi_{\mathcal{K}}$, which would simply follow by the observation that $\mathcal{S}$ is a linear subspace of $\mathbb{R}^{n\times n}$ and Pythagoras' theorem. However, we will need the variational formulation (4) to reduce a bilevel optimization problem to a single-level one at the end of Section 3.

Corollary 2.7 *Let $\mathcal{K} \subseteq \mathcal{S}_n$ be a closed convex cone. If $\mathsf{X} \in \overline{\mathcal{K}}$, then $\Pi_{\mathcal{K}}\mathsf{X} = \bar{\mathsf{X}}$.*

Proof If $\bar{\mathsf{X}} \in \mathcal{K}$, then $\mathsf{C} = \mathsf{O}$ and $\mathsf{Y} = \bar{\mathsf{X}}$ satisfy the conditions in Theorem 2.6. □

Corollary 2.8 *Let $\mathsf{X} \in \mathbb{R}^{n\times n}$. We have the following projection formulae:*

(a) $\Pi_{\mathcal{S}}\mathsf{X} = \bar{\mathsf{X}} := \frac{1}{2}(\mathsf{X} + \mathsf{X}^\top)$,
(b) $\Pi_{\mathcal{N}}\mathsf{X} = \bar{\mathsf{X}}_+ := [(\bar{X}_{ij})_+]_{i,j}$, *the entrywise truncation of $\bar{\mathsf{X}}$ to $\mathbb{R}_+$,*
(c) $\Pi_{\mathcal{S}^+}\mathsf{X} = \mathsf{T}\mathsf{D}_+\mathsf{T}^\top$, where $\bar{\mathsf{X}} = \mathsf{T}\mathsf{D}\mathsf{T}^\top$ is the spectral decomposition of $\bar{\mathsf{X}}$ with orthonormal $\mathsf{T} \in \mathbb{R}^{n\times n}$ and $\mathsf{D} = \mathrm{Diag}(\lambda_1, \ldots, \lambda_n)$ the diagonal matrix containing the eigenvalues of $\bar{\mathsf{X}}$.

Proof This follows from Theorem 2.6 by verifying that the matrix C resulting from formula (3) fulfills $\mathsf{C} \in \mathcal{K}^*$ and $\mathsf{C} \perp \mathsf{Y} = \bar{\mathsf{X}} + \mathsf{C} \in \mathcal{K}$ for the given cones $\mathcal{K}$. Observe that $\mathcal{S}^* = \{\mathsf{O}\}$ in case (a), and use the self-duality for the cones $\mathcal{N}$ and $\mathcal{S}^+$ in cases (b) and (c). □

3 A Nonsymmetric CP-Rank

A well-known concept in Nonnegative Matrix Factorization (NMF, cf. [13]) is that of the *nonnegative rank* of a (possibly rectangular) nonnegative matrix $\mathsf{A} \in \mathbb{R}^{m\times n}_+$:

$$\mathrm{rank}_+(\mathsf{A}) := \min\{r \in \mathbb{N} : \mathsf{A} = \mathsf{L}\mathsf{R}, \mathsf{L} \in \mathbb{R}^{m\times r}_+, \mathsf{R} \in \mathbb{R}^{r\times n}_+\}.$$

Obviously, we have

$$\mathrm{rank}(\mathsf{A}) = \mathrm{rank}(\mathsf{A}^\top) \leq \mathrm{rank}_+(\mathsf{A}) = \mathrm{rank}_+(\mathsf{A}^\top) \leq \min\{m, n\},$$

with strictness possible for the leftmost inequality if $\min(m, n) \geq 4$ (cf. [24]), or for the pathological case $\mathsf{A} = \mathsf{O} \in \mathbb{R}^{m\times n}$ of any size.

Returning to the case of square matrices $\mathsf{X} \in \mathbb{R}^{n\times n}_+$, first recall the definition of the usual (symmetric) *cp-rank* for $\mathsf{C} \in \mathcal{CP}_n \subset \mathcal{S}_n$:

$$\mathrm{cpr}(\mathsf{C}) := \inf\{r \in \mathbb{N} : \mathsf{C} = \mathsf{F}^\top\mathsf{F}, \mathsf{F} \in \mathbb{R}^{r\times n}_+\}.$$

We have $\mathrm{rank}_+(\mathsf{C}) \leq \mathrm{cpr}(\mathsf{C})$, and a significant difference is possible as cpr may increase quadratically with the order of C while rank_+ is bounded above by the order. Note that for $\mathsf{C} \in \mathcal{N}_n \setminus \mathcal{CP}_n$, we have $\mathrm{rank}_+(\mathsf{C}) \leq n < +\infty = \mathrm{cpr}(\mathsf{C})$, extending the definition of $\mathrm{cpr}(\mathsf{C})$ consistently with usual default regulations for infima.

Now we consider a seemingly new variant of this concept for the nonsymmetric case. This is motivated by the fact that all previously discussed matrix parameters, $\mathrm{rank}\,\mathsf{X}$ and $\mathrm{rank}_+\mathsf{X}$, are defined for nonsymmetric square matrices X as well. Imitating the low-rank NMF approach, we assign a *nonsymmetric cp-rank* to these $\mathsf{X} \in \mathbb{R}^{n\times n}_+$ as follows:

For any $r \in \mathbb{N}$, define

$$\delta_r(\mathsf{X}) := \min\{\|\mathsf{X} - \mathsf{Y}\| : \mathsf{Y} \in \mathcal{S}_n, \mathrm{cpr}(\mathsf{Y}) \leq r\} \geq 0,$$

and observe that $\delta_r(\mathsf{X})$ is non-increasing with r for any $\mathsf{X} \in \mathbb{R}^{n\times n}$. The minimum exists since it is attained in a closed set inside a ball of radius, say, $2\|\mathsf{X}\| + 1$.

Now either use, as in determining the cluster number, an elbow criterion on the sequence $\{\delta_r(\mathsf{X}) : r \in \mathbb{N}\}$ to determine an analogue or even, more boldly, ask for exact stabilization via the definition

$$\overline{\mathrm{cpr}}(\mathsf{X}) := \min\{r \in \mathbb{N} : \delta_r(\mathsf{X}) = \delta_s(\mathsf{X}) \text{ for all } s \geq r\}.$$

Theorem 3.1 *Let* $\mathsf{Y} := \Pi_{\mathcal{CP}}\mathsf{X}$ *be the minimal distance projection of* X *onto the closed convex cone* $\mathcal{CP}$. *Then* $\overline{\mathrm{cpr}}(\mathsf{X}) = \mathrm{cpr}(\mathsf{Y})$.

Proof For $r := \mathrm{cpr}(\mathsf{Y}) \in \mathbb{N}$ we have

$$\delta_{r-1}(\mathsf{X}) > \delta_s(\mathsf{X}) \quad \text{for all } s \geq r,$$

since equality above would conflict with minimality of $r = \mathrm{cpr}(\mathsf{Y})$ and the uniqueness of $\Pi_{\mathcal{CP}}\mathsf{X} = \mathsf{Y}$. Hence $\overline{\mathrm{cpr}}(\mathsf{X}) = \mathrm{cpr}(\mathsf{Y}) = r$ with $\delta_r(\mathsf{X}) = \|\mathsf{X} - \mathsf{Y}\|$. □

Let us look at $\Pi_{\mathcal{CP}}\mathsf{X}$ in the case that $\mathsf{X} \in \overline{\mathcal{CP}}$:

Corollary 3.2 *Let* $\mathsf{X} \in \overline{\mathcal{CP}} \setminus \mathcal{S}$. *Then* $\Pi_{\mathcal{CP}}\mathsf{X} = \Pi_{\mathcal{S}}\mathsf{X} = \frac{1}{2}(\mathsf{X}+\mathsf{X}^\top) = \bar{\mathsf{X}}$, *and for* $r := \mathrm{cpr}(\bar{\mathsf{X}}) \in \mathbb{N}$ *we have*

$$\delta_{r-1}(\mathsf{X}) > \delta_s(\mathsf{X}) = \|\mathsf{X} - \Pi_{\mathcal{CP}}\mathsf{X}\| = \tfrac{1}{2}\|\mathsf{X} - \mathsf{X}^\top\| > 0 \;\; \textit{for all } s \geq r.$$

Hence $\overline{\mathrm{cpr}}(\mathsf{X}) = \mathrm{cpr}(\bar{\mathsf{X}})$ *for all* $\mathsf{X} \in \overline{\mathcal{CP}}$.

Proof Apply Corollary 2.7 to $\mathcal{K} = \mathcal{CP}$ and use Theorem 3.1. For any $s \geq r = \mathrm{cpr}(\bar{\mathsf{X}})$, we conclude that $\delta_s(\mathsf{X}) = \delta_r(\mathsf{X}) < \delta_{r-1}(\mathsf{X})$ and hence $\overline{\mathrm{cpr}}(\mathsf{X}) = r = \mathrm{cpr}(\bar{\mathsf{X}})$. □

Example 3.3 Consider

$$\mathsf{X} = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} \in \overline{\mathcal{CP}_2}.$$

We have $\mathrm{rank}_+(\mathsf{X}) = \mathrm{rank}(\mathsf{X}) = 2$, but $\overline{\mathrm{cpr}}(\mathsf{X}) = \mathrm{cpr}(\bar{\mathsf{X}}) = \mathrm{cpr}(\mathbf{ee}^\top) = 1$ with $\delta_1(\mathsf{X}) = \sqrt{2}$.

Example 3.4 Consider

$$\mathsf{X} = \begin{bmatrix} 2 & 1 \\ 0 & 2 \end{bmatrix} \in \overline{\mathcal{CP}_2}.$$

We have $\delta_1(\mathsf{X}) = \frac{\sqrt{11}}{2} \approx 1.66$. Here $\mathrm{rank}_+(\mathsf{X}) = \mathrm{rank}(\mathsf{X}) = 2$ and $\overline{\mathrm{cpr}}(\mathsf{X}) = \mathrm{cpr}(\bar{\mathsf{X}}) = \mathrm{rank}(\bar{\mathsf{X}}) = 2$ with $\delta_2(\mathsf{X}) = \frac{1}{\sqrt{2}} \approx 0.71$.

Example 3.5 For

$$\mathsf{X} = \begin{bmatrix} 0 & 3 \\ -1 & 1 \end{bmatrix} \in \mathbb{R}^{2\times 2} \setminus (\overline{\mathcal{CP}_2} \cup \mathbb{R}^{2\times 2}_+)$$

we have $\bar{\mathsf{X}} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \in \mathcal{N}_2 \setminus \mathcal{CP}_2$ with $\|\mathsf{X} - \Pi_{\mathcal{S}}\mathsf{X}\| = \sqrt{8}$. Now let $t := \frac{1+\sqrt{5}}{2} > 1$ be the larger root of the Golden Section/Fibonacci polynomial $t^2 - t - 1$ and define

$$\mathsf{Y} := \frac{t}{2+t}\begin{bmatrix} 1 & t \\ t & t^2 \end{bmatrix} \quad \text{and} \quad \mathsf{C} := \frac{1}{2+t}\begin{bmatrix} t & -1 \\ -1 & t-1 \end{bmatrix}.$$

It is easy to verify that $\mathsf{Y} \in \mathcal{CP}_2$ and $\mathsf{C} \in \mathcal{S}_2^+ \subset \mathcal{COP}_2 = \mathcal{CP}_2^*$, as well as $\mathsf{C} \perp \mathsf{Y}$. Furthermore, we have $\mathsf{Y} = \bar{\mathsf{X}} + \mathsf{C}$, and hence by Theorem 2.6 we get

$$\Pi_{\mathcal{CP}}\mathsf{X} = \mathsf{Y} = \frac{1}{2\sqrt{5}}\begin{bmatrix} 2 & 1+\sqrt{5} \\ 1+\sqrt{5} & 3+\sqrt{5} \end{bmatrix},$$

with $\overline{\text{cpr}}(\mathsf{X}) = \text{cpr}\mathsf{Y} = 1$ and (note that $\Pi_{\mathcal{CP}}\mathsf{X} \neq \mathbf{e}\mathbf{e}^\top = \bar{\mathsf{X}} + \mathbf{e}_1\mathbf{e}_1^\top \in \mathcal{CP}_2$)

$$\|\mathsf{X} - \mathbf{e}\mathbf{e}^\top\|^2 = 9 > \delta_1^2(\mathsf{X}) = 9 - \frac{t}{5(t+1)} = \frac{3-\sqrt{5}}{5} > 8 = \|\mathsf{X} - \bar{\mathsf{X}}\|^2.$$

The calculation of $\overline{\text{cpr}}(\mathsf{X})$ according to its definition amounts to solving a bilevel minimization problem, namely

$$\overline{\text{cpr}}(\mathsf{X}) = \min\{r : \mathsf{Y} = \mathsf{F}^\top\mathsf{F}\,,\ \mathsf{F} \in \mathbb{R}_+^{r\times n},\ \|\mathsf{Y} - \bar{\mathsf{X}}\| = \min\{\|\mathsf{Z} - \bar{\mathsf{X}}\| : \mathsf{Z} \in \mathcal{CP}_n\}\},$$

which is hard by structure even we ignore the hardness of the conic constraints $\{\mathsf{Y}, \mathsf{Z}\} \subset \mathcal{CP}_n$ due to the general hardness of bilevel optimization and the non-convex quadratic constraint $\mathsf{F}^\top\mathsf{F} = \mathsf{Y}$. The above problem has the integer variable $r \in \mathbb{N}$ plus many continuous variables, namely all entries in Y and F. By minimality of r, no row $\mathbf{f}_i^\top$ of F can be zero.

Instead, we can always add zero rows to F until we reach the upper bound $p = p_n := \binom{n+1}{2} - 4$ on $\text{cpr}(\mathsf{Y})$ over $\mathsf{Y} \in \mathcal{CP}_n$, and then minimize the number of non-zero rows of F to achieve minimality of r. Since all $\mathbf{f}_i \in \mathbb{R}_+^n$, we have $\mathbf{f}_i \neq \mathbf{o}$ if and only if $\mathbf{e}^\top\mathbf{f}_i > 0$, so this count exactly amounts to the zero (pseudo-)norm

$$\|\mathsf{F}\mathbf{e}\|_0 := |\{i \in \{1, \ldots, p\} : \mathbf{e}_i^\top\mathsf{F}\mathbf{e} > 0\}|.$$

The zero norm $\|\cdot\|_0$ is discontinuous and therefore not directly tractable in a minimization problem. However, as shown by several authors [5, 7, 10, 12, 27], there is a continuous QCQP reformulation for the minimization of a zero norm which blends well into the framework of copositive optimization:

Theorem 3.6 *Let $\mathsf{X} \in \mathbb{R}^{n\times n}$, let $p = p_n = \binom{n+1}{2} - 4$, and denote $\mathbf{e} \in \mathbb{R}^n$ and $\bar{\mathbf{e}} \in \mathbb{R}^p$. Then*

$$\overline{\text{cpr}}(\mathsf{X}) = p - \max_{\mathbf{u},\mathsf{F},\mathsf{C}}\Big\{\bar{\mathbf{e}}^\top\mathbf{u} :\ \mathbf{u}^\top\mathsf{F}\mathbf{e} = 0,\ \mathsf{F}^\top\mathsf{F} = \mathsf{C} + \bar{\mathsf{X}},\ \langle\mathsf{C}, \mathsf{C} + \bar{\mathsf{X}}\rangle = 0,$$
$$\mathbf{u} \in [0,1]^p,\ \mathsf{F} \in \mathbb{R}_+^{p\times n},\ \mathsf{C} \in \mathcal{COP}_n\Big\},$$

a conic QCQP over the copositive cone with $\mathcal{O}(n^3)$ continuous variables and $\mathcal{O}(n^2)$ constraints.

Proof As in [5, 7], we argue that the minimal zero norm over a feasible set $\mathcal{F} \subseteq \mathbb{R}_+^p$ is given by the solution to a complementarity-constrained problem over the same set $\mathcal{F}$:

$$\min\{\|\mathbf{v}\|_0 : \mathbf{v} \in \mathcal{F}\} = \min\{\bar{\mathbf{e}}^\top(\bar{\mathbf{e}} - \mathbf{u}) : \mathbf{u}^\top\mathbf{v} = 0,\ \mathbf{u} \in [0,1]^p,\ \mathbf{v} \in \mathcal{F}\}.$$

Indeed, optimality in the above problem forces all u_i to be binary, and then $\bar{\mathbf{e}}^\top(\bar{\mathbf{e}} - \mathbf{u})$ counts the non-zero entries of $\mathbf{v}$. If $\mathbf{v} = \mathsf{F}\mathbf{e}$ for some $\mathsf{F} \in \mathbb{R}_+^{p\times n}$, then $\|\mathbf{v}\|_0$ counts the non-zero rows of F, and its minimal value equals $\text{cpr}(\mathsf{Y})$ if F ranges over all these matrices subject to the quadratic constraints $\mathsf{F}^\top\mathsf{F} = \mathsf{Y}$, which we write as $\mathsf{Y} = \mathsf{C} + \bar{\mathsf{X}}$. The claim now follows from the variational characterization of $\Pi_{\mathcal{CP}}\mathsf{X}$ in Theorem 2.6 and from Theorem 3.1. □

4 Copositive-plus Results

Recall that a (possibly nonsymmetric) square matrix $\mathsf{Q} \in \mathbb{R}^{n\times n}$ is said to be *copositive-plus*, if $\mathsf{Q} \in \overline{\mathcal{COP}_n}$ and if $\mathbf{x}^\top \mathsf{Q}\mathbf{x} = 0$ with $\mathbf{x} \in \mathbb{R}^n_+$ implies $\mathsf{Q}\mathbf{x} = \mathbf{o}$. In other words, Q is copositive-plus if $\min\{\mathbf{x}^\top \mathsf{Q}\mathbf{x} : \mathbf{x} \in \Delta^n\} \geq 0$ and the *set of zeroes*

$$Z(\mathsf{Q}) := \{\mathbf{x} \in \Delta^n : \mathbf{x}^\top \mathsf{Q}\mathbf{x} = 0\}$$

can be expressed as $Z(\mathsf{Q}) = \Delta^n \cap \operatorname{Ker} \mathsf{Q}$. If $Z(\mathsf{Q}) = \emptyset$, then $\mathsf{Q} \in \overline{\mathcal{COP}_n}$ is called *strictly copositive*. Otherwise, if Q is copositive-plus, then $Z(\mathsf{Q})$ is a polytope and hence a convex set. This implies that any finite, non-singleton $Z(\mathsf{Q})$ certifies that Q is not copositive-plus. An example for this is $\mathsf{Q} = \mathbf{e}\mathbf{e}^\top - \mathsf{I}_n$ with $Z(\mathsf{Q}) = \{\mathbf{e}_i : i \in \{1, \dots, n\}\}$.

Remark 4.1 An alternative definition of a copositive-plus matrix can be found in the very informative survey [8] where $\mathsf{Q} \in \overline{\mathcal{COP}_n}$ is defined to be copositive-plus if $\mathbf{x} \in Z(\mathsf{Q})$ implies $(\mathsf{Q} + \mathsf{Q}^\top)\mathbf{x} = \mathbf{o}$, or

$$Z(\mathsf{Q}) = \Delta^n \cap \operatorname{Ker}(\overline{\mathsf{Q}}).$$

This definition obviously differs from ours (which seems to be widely accepted in the community now), and will not be used in the sequel. However, the attentive reader will notice that some of our results below actually are related to this variant. To avoid confusion, we will stick to the first definition, so $Z(\mathsf{Q}) = \Delta^n \cap \operatorname{Ker} \mathsf{Q}$ and **not** $Z(\mathsf{Q}) = \Delta^n \cap \operatorname{Ker}(\overline{\mathsf{Q}})$. This approach seems more transparent, even if it may require a few slightly lengthier formulations.

Theorem 4.2 *If* $\mathsf{Q} \in \mathbb{R}^{n\times n}$ *generates a quadratic form taking no negative values over a neighborhood* $U \subset H$ *of* Δ^n *relative to the supporting hyperplane* $H := \mathbf{e}^\perp + \frac{1}{n}\,\mathbf{e} = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{e}^\top \mathbf{x} = 1\}$, *then* $\mathsf{Q} + \mathsf{Q}^\top$ *is copositive-plus.*

Proof By homogeneity it is immediate that Q and $\mathsf{Q} + \mathsf{Q}^\top$ are copositive (over $\mathbb{R}^n_+$). Now suppose that $\mathbf{x}^\top \mathsf{Q}\mathbf{x} = 0$ for some $\mathbf{x} \in \Delta^n$ and consider $\mathbf{q} := (\mathsf{Q} + \mathsf{Q}^\top)\mathbf{x}$ as well as a step size $t > 0$ so small that $\mathbf{e}^\top(\mathbf{x} - t\mathbf{q}) \in [\frac{1}{2}, 2]$. Then

$$\mathbf{y}_t := \frac{1}{\mathbf{e}^\top(\mathbf{x} - t\mathbf{q})}\,(\mathbf{x} - t\mathbf{q}) \in U$$

if t is small enough, because $\mathbf{y}_t \to \mathbf{x}$ as $t \searrow 0$. By assumption, we get $\mathbf{y}_t^\top \mathsf{Q}\mathbf{y}_t \geq 0$ and hence

$$\begin{aligned} 0 &\leq [\mathbf{e}^\top(\mathbf{x} - t\mathbf{q})]^2 \mathbf{y}_t^\top \mathsf{Q}\mathbf{y}_t \\ &\leq 4[\mathbf{x}^\top \mathsf{Q}\mathbf{x} - t\mathbf{q}^\top(\mathsf{Q}\mathbf{x} + \mathsf{Q}^\top\mathbf{x}) + t^2\mathbf{q}^\top \mathsf{Q}\mathbf{q}] \\ &= 4t[-\|\mathbf{q}\|^2 + t\mathbf{q}^\top \mathsf{Q}\mathbf{q}], \end{aligned}$$

which for small enough $t > 0$ implies that $\|\mathbf{q}\| \leq 0$, so $(\mathsf{Q} + \mathsf{Q}^\top)\mathbf{x} = \mathbf{q} = \mathbf{o}$ and hence $\mathsf{Q} + \mathsf{Q}^\top$ is copositive-plus. □

We now consider a specific family of neighborhoods of Δ^n relative to H.

Theorem 4.3 *Let* $\delta \in (0, 1)$ *and define*

$$U_\delta := \operatorname{conv}\left\{(1 + \delta)\mathbf{e}_i - \frac{\delta}{n}\,\mathbf{e} : i = 1, \dots, n\right\},$$

as well as the cone $\Gamma_\delta := \mathbb{R}_+ U_\delta$. *If, for any* $\delta > 0$, *the matrix* Q *is* Γ_δ*-copositive,* i.e., *if*

$$\mathbf{x}^\top \mathsf{Q}\mathbf{x} \geq 0 \quad \textit{for all } \mathbf{x} \in \Gamma_\delta,$$

then $\mathsf{Q} + \mathsf{Q}^\top$ *is copositive-plus.*

Proof Any Euclidean ε-neighborhood U of Δ^n relative to H satisfies $U \subseteq U_\delta$ for $\varepsilon = \frac{\delta}{n}$. Indeed, if $\mathbf{y} \in H$ with $\|\mathbf{y} - \mathbf{x}\| \leq \varepsilon$ for some $\mathbf{x} \in \Delta^n$, then

$$y_i - 0 \geq y_i - x_i \geq -\|\mathbf{y} - \mathbf{x}\| \geq -\varepsilon$$

implies $y_i \geq -\varepsilon$ and $y_i + \frac{\delta}{n} \geq 0$ whenever $\varepsilon \leq \frac{\delta}{n}$. We conclude that

$$\mathbf{y} = \sum_i y_i \mathbf{e}_i = \sum_i \frac{y_i + \frac{\delta}{n}}{1+\delta} \left[(1+\delta)\mathbf{e}_i - \tfrac{\delta}{n}\mathbf{e}\right] \in U_\delta .$$

Thus the family $\{U_\delta : \delta > 0\}$ constitutes a neighborhood base of Δ^n relative to H. The claim now follows from Theorem 4.2. □

Using barycentric coordinates it is easy to see that Γ_δ-copositivity of Q can be equivalently formulated as classical $\mathbb{R}^n_+$-copositivity of

$$\mathsf{Q}_\delta := \mathsf{F}_\delta^\top \mathsf{Q} \mathsf{F}_\delta \quad \text{with} \quad \mathsf{F}_\delta := (1+\delta)\, \mathsf{I}_n - \frac{\delta}{n} \mathbf{e}\mathbf{e}^\top . \tag{6}$$

Corollary 4.4 *Any* $\mathsf{Q} \in \mathcal{COP}_n$ *with* $\mathsf{Q}\mathbf{e} = \mathbf{o}$ *is copositive-plus.*

Proof Observe from (6) that $\mathsf{Q}\mathbf{e} = \mathbf{o}$ implies $\mathsf{Q}_\delta = (1+\delta)^2 \mathsf{Q} \in \mathcal{COP}_n$, so that Q is Γ_δ-copositive for all $\delta > 0$. The result follows by Theorem 4.3. □

Remark 4.5 An alternative proof of Corollary 4.4 would employ the observation that for $\mathsf{Q} \in \mathcal{COP}_n$, any $\mathbf{x} \in Z(\mathsf{Q})$ satisfies the first-order condition $\mathsf{Q}\mathbf{x} \in \mathbb{R}^n_+$ necessary [16, 25] for minimality of $\mathbf{x}^\top \mathsf{Q} \mathbf{x}$ over Δ^n, hence $0 \leq \mathbf{e}^\top \mathsf{Q}\mathbf{x} = (\mathsf{Q}\mathbf{e})^\top \mathbf{x} = \mathbf{o}^\top \mathbf{x} = 0$, implying $\mathsf{Q}\mathbf{x} = \mathbf{o}$. But we get even more in a direct way: we have $\sigma(\mathbf{e}) = \{1, \ldots, n\}$ so that Q must be positive-semidefinite by the second-order necessary optimality condition (this time for $\mathbf{x} = \mathbf{e}$), and therefore copositive-plus. Anyhow, Proposition 4.9 below would also yield $\mathsf{Q} \in \mathcal{S}^+_n$ from the assumptions.

On the other hand, if all row sums of Q are positive, i.e., if

$$(\mathsf{Q}\mathbf{e})_i \geq \alpha > 0 \quad \text{for all } i, \tag{7}$$

then Γ_δ-copositivity conflicts with extremality in the cone $\mathcal{COP}$:

Proposition 4.6 *Suppose that the matrix* $\mathsf{Q} \in \mathcal{S}_n$ *satisfies (7) and is* Γ_δ*-copositive for some* $\delta > 0$. *Then* Q *is strictly copositive and thus cannot generate an extremal ray of* $\mathcal{COP}_n$.

Proof For Q_δ as defined in (6), we calculate

$$\mathsf{Q}_\delta = (1+\delta)^2 \mathsf{Q} - \tfrac{\delta}{n}[\mathbf{e}(\mathsf{Q}\mathbf{e})^\top + (\mathsf{Q}\mathbf{e})\mathbf{e}^\top] + \tfrac{\delta^2}{n^2}(\mathbf{e}^\top \mathsf{Q}\mathbf{e})\mathbf{e}\mathbf{e}^\top = (1+\delta)^2 \mathsf{Q} - \tfrac{\delta}{n}\mathsf{C},$$

where

$$\mathsf{C} = \mathbf{e}\mathbf{e}^\top \mathsf{Q} + \mathsf{Q}\mathbf{e}\mathbf{e}^\top - \tfrac{\delta}{n}(\mathbf{e}^\top \mathsf{Q}\mathbf{e})\mathbf{e}\mathbf{e}^\top \in \mathcal{S}_n .$$

For any $\mathbf{x} \in \Delta^n$ we have by (7) that

$$\mathbf{x}^\top \mathsf{C}\mathbf{x} = 2(\mathsf{Q}\mathbf{e})^\top \mathbf{x} - \tfrac{\delta}{n}(\mathbf{e}^\top \mathsf{Q}\mathbf{e}) \geq 2\alpha - \tfrac{\delta}{n}(\mathbf{e}^\top \mathsf{Q}\mathbf{e}) > 0$$

for any δ with $0 < \delta < \frac{2n\alpha}{\mathbf{e}^\top \mathsf{Q}\mathbf{e}}$, and therefore C is strictly copositive. Obviously, the same holds for $\mathsf{Q} = (1+\delta)^{-2}[\mathsf{Q}_\delta + \frac{\delta}{n}\mathsf{C}]$. □

The converse holds without any assumptions like (7):

Theorem 4.7 *If* Q *is strictly copositive, then there exists a* $\delta > 0$ *such that* Q *is* Γ_δ*-copositive.*

Proof If Q is strictly copositive, then the value

$$\min\{\mathbf{x}^\top \mathsf{Q}\mathbf{x} : \mathbf{x} \in \Delta^n\}$$

is strictly positive. By standard continuity and compactness arguments, the same holds true for a small enough neighborhood U of Δ^n relative to H. The result follows from the observations proving Theorem 4.3 and the definition $\Gamma_\delta = \mathbb{R}_+ U_\delta$. □

Any positive-semidefinite matrix Q generating a quadratic form which is zero at some point in Δ^n (also $\mathsf{Q} = \mathsf{O}$) is an example of the fact that the converse of Theorem 4.7 does not hold. Moreover, it is evident that strict copositivity of a nonsymmetric matrix Q by default implies that both Q and $\mathsf{Q}^\top$ are copositive-plus.

However, this is not guaranteed by Γ_δ-copositivity of a nonsymmetric Q, i.e., the nonsymmetric counterpart of Theorem 4.3 is not true. To see this, consider the matrix

$$\mathsf{Q} = \begin{bmatrix} 1 & -2 \\ 0 & 1 \end{bmatrix}.$$

Since $\mathsf{Q}+\mathsf{Q}^\top \in \mathcal{S}_2^+$, it follows that Q is Γ_δ-copositive, and of course $\mathsf{Q}+\mathsf{Q}^\top$ is copositive-plus. On the other hand, Q itself is not copositive-plus since for $\mathbf{x}^\top = [1, 1]$, we have $\mathbf{x}^\top \mathsf{Q}\mathbf{x} = 0$, but $\mathsf{Q}\mathbf{x} \neq \mathbf{o}$.

The converse of Theorem 4.3 is true on the subcone $\mathcal{S}^+ + \mathcal{N} \subseteq \mathcal{COP}$:

Theorem 4.8 *If* $\mathsf{Q} \in \overline{\mathcal{S}_n^+ + \mathcal{N}_n}$ *is copositive-plus, then for all sufficiently small* $\delta > 0$*, the (possibly nonsymmetric) matrix* Q *is* Γ_δ*-copositive.*

Proof Suppose $\mathsf{Q} + \mathsf{Q}^\top = \mathsf{S} + \mathsf{N}$ with $\mathsf{S} \in \mathcal{S}_n^+$ and $\mathsf{N} \in \mathcal{N}_n$. Obviously, S is copositive-plus, so $\mathsf{Q} + \mathsf{Q}^\top$ is copositive-plus if and only if N is so. But then a zero on the diagonal forces the whole column of N to zero: if $0 = \mathbf{e}_i^\top \mathsf{N}\mathbf{e}_i = N_{ii}$, then $\mathsf{N}\mathbf{e}_i = \mathbf{o}$, cf. [26]. Hence we may decompose

$$\mathsf{N} = \begin{bmatrix} \mathsf{R} & \mathsf{O} \\ \mathsf{O}^\top & \mathsf{O} \end{bmatrix},$$

where $\mathsf{R} \in \mathcal{N}_k$ has a strictly positive diagonal and therefore is strictly copositive ($k = 0$ is possible but then $\mathsf{N} = \mathsf{O}$ and nothing remains to be shown). Decomposing $\mathbf{x}^\top = [\mathbf{u}^\top | \mathbf{v}^\top]$ with $\mathbf{u} \in \mathbb{R}^k$, we arrive at

$$2\mathbf{x}^\top \mathsf{Q}\mathbf{x} = \mathbf{x}^\top \mathsf{S}\mathbf{x} + \mathbf{u}^\top \mathsf{R}\mathbf{u} \geq \mathbf{u}^\top \mathsf{R}\mathbf{u} > 0 \quad \text{if } \mathbf{u} \text{ is close enough to } \Delta^k,$$

arguing by equicontinuity as above, which establishes Γ_δ-copositivity of Q, as claimed. □

It is an open question whether there are exceptional copositive-plus matrices. The simplest candidate would be the Horn matrix [21], denoted by $\mathsf{H} \in \mathcal{COP}_5$. However, H is not copositive-plus, as $\mathbf{x}^\top = [2, 1, 0, 0, 1]$ gives $\mathsf{H}\mathbf{x} = [0, 0, 2, 2, 0]$ and $\mathbf{x}^\top \mathsf{H}\mathbf{x} = 0$. The following result is more general:

Proposition 4.9 *Let* $\mathsf{Q} \in \mathcal{COP}_n$ *be copositive-plus and let* $Z(\mathsf{Q}) = \operatorname{Ker} \mathsf{Q} \cap \Delta^n$*. If*

$$\bigcup\{\sigma(\mathbf{x}) : \mathbf{x} \in Z(\mathsf{Q})\} = \{1, \ldots, n\}, \tag{8}$$

then $\mathsf{Q} \in \mathcal{S}_n^+$ *and thus is* Γ_δ*-copositive for all* $\delta > 0$.

Proof If (8) holds, then $Z(\mathsf{Q}) \neq \emptyset$, so $Z(\mathsf{Q})$ is a convex set, and thus the assumptions imply existence of $\bar{\mathbf{x}} \in Z(\mathsf{Q})$ with $\min_i \bar{x}_i > 0$ in the relative interior of Δ^n. Now consider any $\mathbf{y} \in (\operatorname{Ker}\mathsf{Q})^\perp = \mathsf{Q}(\mathbb{R}^n)$. For sufficiently small $|t| > 0$, we have $\bar{\mathbf{x}} + t\mathbf{y} \in \mathbb{R}^n_+$ and thus, by copositivity of Q,

$$0 \le (\bar{\mathbf{x}} + t\mathbf{y})^\top \mathsf{Q}(\bar{\mathbf{x}} + t\mathbf{y}) = t^2\mathbf{y}^\top \mathsf{Q}\mathbf{y}.$$

For any $\mathbf{x} \in \mathbb{R}^n$, consider now the unique decomposition $\mathbf{x} = \mathbf{u} + \mathbf{y}$ with $\mathbf{u} \in \operatorname{Ker}\mathsf{Q}$ and $\mathbf{y} \perp \operatorname{Ker}\mathsf{Q}$. We obtain from $\mathbf{y}^\top \mathsf{Q}\mathsf{y} \ge 0$ that

$$\mathbf{x}^\top \mathsf{Q}\mathbf{x} = \mathbf{u}^\top \mathsf{Q}\mathbf{u} + 2\mathsf{y}^\top \mathsf{Q}\mathbf{u} + \mathbf{y}^\top \mathsf{Q}\mathsf{y} = \mathbf{y}^\top \mathsf{Q}\mathbf{y} \ge 0,$$

which establishes $\mathsf{Q} \in \mathcal{S}_n^+$. □

Remark 4.10 Let us discuss exceptional copositive-plus matrices on the boundary of the copositive cone which have a zero $\mathbf{x} \in Z(\mathsf{Q})$. Proposition 4.9 implies $\sigma(\mathbf{x}) \neq \{1, \dots, n\}$. Without loss of generality, assume $\sigma(\mathbf{x}) = \{1, \dots, k\}$ for some $k < n$. As is well known [15], in this case Q and $\mathbf{x}$ can be decomposed as

$$\mathsf{Q} = \begin{bmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{B}^\top & \mathsf{C} \end{bmatrix} \quad \text{and} \quad \mathbf{x} = \begin{bmatrix} \mathbf{y} \\ \mathbf{o} \end{bmatrix}$$

with $\mathbf{y} \in \Delta^k$, $\mathsf{A} \in \mathcal{S}_k^+$ and $\mathsf{A}\mathbf{y} = \mathbf{o}$. But Q is copositive-plus, so $\mathsf{Q}\mathbf{x} = \mathbf{o}$, which implies $\mathsf{B}^\top \mathbf{y} = \mathbf{o}$. However, the first-order KKT condition necessary for optimality of $\mathbf{x}$ in the problem $\min\{\mathbf{z}^\top \mathsf{Q}\mathbf{z} : \mathbf{z} \in \Delta^n\}$ read $\mathsf{A}\mathbf{y} = \mathbf{o}$ and $\mathsf{B}^\top \mathbf{y} \ge \mathbf{o}$, so equality in the latter system signifies a massive departure from strict complementarity.

So, on the boundary of the copositive cone outside $\mathcal{S}^+ + \mathcal{N}$, copositive-plusness implies a sort of degeneracy. Moreover, extremal rays of this cone, if exceptional, can neither be copositive-plus:

Corollary 4.11 *No exceptional extreme copositive matrix* $\mathsf{Q} \in \mathcal{S}_n$ *can be copositive-plus.*

Proof [2, Corollary 3.6] shows that any extreme copositive matrix Q satisfies (8). If Q were copositive-plus, Proposition 4.9 would yield $\mathsf{Q} \in \mathcal{S}_n^+$, in contradiction to exceptionality. □

Corollary 4.12 *Any exceptional matrix* $\mathsf{Q} \in \mathcal{COP}_5$ *which is not strictly copositive and has more than one zero in* $Z(\mathsf{Q})$ *cannot be copositive-plus.*

Proof If $Z(\mathsf{Q})$ is nonconvex (e.g., finite and not a singleton), then Q cannot be copositive-plus. We will show this for exceptional matrices of order 5. Indeed, Q must be a convex combination of extreme matrices where at least one of which, say $\mathsf{R} \in \mathcal{COP}_5$, is exceptional. But then $Z(\mathsf{Q}) \subseteq Z(\mathsf{R})$, and the set $Z(\mathsf{R})$ is known to be finite [14, Theorem 2.3] for all exceptional extremal $\mathsf{R} \in \mathcal{COP}_5 \setminus \mathcal{H}$, where $\mathsf{H} \in \mathcal{COP}_5$ denotes the Horn matrix and

$$\mathcal{H} = \{\mathsf{P}^\top \mathsf{DHDP} : \mathsf{P} \text{ a permutation matrix}, \mathsf{D} \in \operatorname{int}\mathcal{S}_5^+ \text{ diagonal}\}$$

is its orbit. While $Z(\mathsf{H})$ is infinite, it is easily shown that $\mathsf{H}\mathbf{x} \neq \mathbf{o}$ for all $\mathbf{x} \in Z(\mathsf{H})$. Now either all exceptional matrices occurring in the convex combination yielding Q are in $\mathcal{H}$, whence also $\mathsf{Q}\mathbf{x} \neq \mathbf{o}$ for some (or actually all) $\mathbf{x} \in Z(\mathsf{Q})$, or there is an exceptional extremal $\mathsf{R} \in \mathcal{COP}_5 \setminus \mathcal{H}$ as above in this convex combination, with finite $Z(\mathsf{R})$. Hence the result. □

As usual, we call $\mathsf{Q} \in \mathcal{COP}_n$ *irreducible w.r.t.* $\mathcal{S}_n^+$, if for all $\mathsf{P} \in \mathcal{S}_n^+ \setminus \{\mathsf{O}\}$ we have $\mathsf{Q} - \mathsf{P} \notin \mathcal{COP}_n$. Nontrivial matrices of this kind again cannot be copositive-plus:

Corollary 4.13 *Suppose that* $\mathsf{Q} \in \mathcal{COP}_n \setminus \{\mathsf{O}\}$ *is* $\mathcal{S}_n^+$*-irreducible. Then* Q *cannot be copositive-plus.*

Proof From [15, Theorem 4.5] we know that span $Z(\mathsf{Q}) = \mathbb{R}^n$, which implies (8). So if Q were copositive-plus, we would infer via Proposition 4.9 that also $\mathsf{Q} \in \mathcal{S}_n^+$, which in view of irreducibility of $\mathsf{Q} \neq \mathsf{O}$ is a contradiction. Hence the result. □

Let us recapitulate our findings in search of a (symmetric) copositive-plus matrix violating the converse of Theorem 4.3 (so far, we have found no such matrix):

Corollary 4.14 *Suppose that* $\mathsf{Q} \in \mathcal{COP}_n$ *is copositive-plus, but that for no* $\delta > 0$, Q *is* Γ_δ*-copositive. Then* $n \geq 5$ *and*

(a) $Z(\mathsf{Q}) \neq \emptyset$,
(b) Q *must be exceptional, but cannot be extreme in* $\mathcal{COP}_n$,
(c) Q *must be* $\mathcal{S}_n^+$*-reducible:* $\mathsf{Q} = \mathsf{P} + \mathsf{R}$ *for some* $\mathsf{P} \in \mathcal{S}_n^+ \setminus \{\mathsf{O}\}$, *some* $\mathsf{R} \in \mathcal{COP}_n$,
(d) *if* $n \in \{5, 6\}$, *then* $Z(\mathsf{Q}) = \{\mathbf{x}\}$ *must be a singleton at the relative boundary of* Δ^n, i.e., $\sigma(\mathbf{x}) \neq \{1, \ldots, n\}$.

Proof For (a), see also Remark 4.10. Only the last statement (d) needs a proof. But this follows as in the proof of Corollary 4.11 from the recent complete enumeration of exceptional extreme rays of $\mathcal{COP}_6$ (and the supports of their zeroes) in [1]. □

Remark 4.15 Note that there are also exceptional extreme rays in $\mathcal{COP}_6$ of the form H padded with an additional row and column of zeroes, for which the same argument as in the case $n = 5$ discussed in the proof of Corollary 4.12 applies. These matrices are the smallest known copositive ones which cannot lie in any of the smaller Parrilo cones $\mathcal{K}_6^{(r)}$, $r \in \{0\} \cup \mathbb{N}$, whereas H itself lies already in $\mathcal{K}_5^{(1)}$ [18, Example 2]. We conclude that copositive-plusness and (in-)approximability are apparently unrelated. For general n, the sequence of Parrilo cones $(\mathcal{K}_n^{(r)})_{r=0}^\infty$ increases and approximates $\mathcal{COP}_n$ as $r \nearrow \infty$ in the sense that the closure of $\bigcup_{r=0}^\infty \mathcal{K}_n^{(r)}$ coincides with $\mathcal{COP}_n$. They are based upon the sum-of-squares approximation hiearchy as follows: as usual, denote by $\mathbb{R}[\mathbf{x}]$ the vector space of all polynomials in $\mathbf{x} \in \mathbb{R}^n$. Those of them which can be written as the sum of squares of other polynomials $s_i(\mathbf{x})$ form a cone denoted by Σ:

$$\Sigma := \left\{ q \in \mathbb{R}[\mathbf{x}] : q = \sum_i s_i^2,\ s_i \in \mathbb{R}[\mathbf{x}] \right\}.$$

Next, for a vector $\mathbf{x} = [x_i] \in \mathbb{R}^n$ define the vector $\mathbf{x}^{[2]} := [x_i^2] \in \mathbb{R}^n$, and for $r \in \{0\} \cup \mathbb{N}$ and $\mathsf{M} \in \mathcal{S}_n$, define the polynomial

$$q_{r,\mathsf{M}}(\mathbf{x}) := (\mathbf{x}^\top \mathbf{x})^r\ (\mathbf{x}^{[2]})^\top \mathsf{M}(\mathbf{x}^{[2]}),\ \mathbf{x} \in \mathbb{R}^n.$$

Finally, define the matrix cone

$$\mathcal{K}_n^{(r)} := \{\mathsf{M} \in \mathcal{S}_n : q_{r,\mathsf{M}} \in \Sigma\}.$$

Since $q_{r+1,\mathsf{M}}(\mathbf{x}) = (\mathbf{x}^\top \mathbf{x})\, q_{r,\mathsf{M}}(\mathbf{x}) = \sum_i (\mathbf{x}^\top \mathbf{x})[s_i(\mathbf{x})]^2 = \sum_{i,j} [x_j s_i(\mathbf{x})]^2$, we have $\mathcal{K}_n^{(r)} \subset \mathcal{K}_n^{(r+1)}$, and by writing $\mathbf{y} = \mathbf{x}^{[2]} \in \mathbb{R}_+^n$ and the definitions, we see that $\mathcal{K}_n^{(r)} \subset \mathcal{COP}_n$ for all r.

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