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THE COPOSITIVE RANGE*

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Abstract. We consider symmetric copositive matrices $A \in \mathbf{M}_n(\mathbb{R})$, which by definition satisfy $x^T Ax \geq 0$ for all nonzero $x \geq 0$. We introduce the notion the copositive range of a copositive matrix A,

$$CR(A) = \{x^T Ax \,:\, x \geq 0,\ \|x\|_2 = 1\},$$

and prove that $CR(A)$ is an interval contained in the numerical range of A. We focus on the properties and the endpoints of $CR(A)$, which are associated with the Pareto eigenvalues of A.

Key words. Copositive matrix, Numerical range, Pareto eigenvalues.

AMS subject classifications. 15A48, 15A57, 15A63, 90C20.

1. Introduction.

Given an $n \times n$ real matrix $A \in \mathbf{M}_n(\mathbb{R})$ and the set $\mathbb{R}^n_+$ of entrywise nonnegative n-vectors, consider the set

$$C_A = \{x \in \mathbb{R}^n_+ \,:\, x^T Ax \geq 0\}.$$

Since $x^T Ax \geq 0$ if and only if $x^T(A + A^T)x \geq 0$, we will focus on C_A for symmetric matrices A. If for all $x \in \mathbb{R}^n_+$, $x^T Ax \geq 0$, then a symmetric $A \in \mathbf{M}_n(\mathbb{R})$ is known as a copositive matrix. That is, a symmetric $A \in \mathbf{M}_n(\mathbb{R})$ is copositive if $C_A = \mathbb{R}^n_+$.

A criterion for a matrix A to be copositive is that no principal submatrix of A can have a positive eigenvector that is associated with a negative eigenvalue [21, Theorem 2]. This criterion generally commands exponential complexity to detect a copositive matrix.

The (symmetric) positive semidefinite matrices and the symmetric (entrywise) nonnegative matrices are indeed among well-known classes of copositive matrices. As a simple consequence, any matrix that is the sum of a positive semidefinite matrix and a symmetric nonnegative matrix is copositive. Copositive matrices that are not such a sum exist [14] and are referred to as *exceptional.* No criterion that can be easily used to identify exceptional copositive matrices is known.

The present paper aims to advance the theory of copositive matrices with the detection and categorization of copositive matrices mentioned above in mind. For that purpose, we introduce and examine the copositive range of a copositive matrix A; that is, the set

$$CR(A) = \{x^T Ax : x \geq 0,\ \|x\|_2 = 1\} \subseteq \mathbb{R}_+.$$

The presentation consists of Section 2 that contains notation, definitions, and a review of basic facts about copositive matrices; for the general theory and applications of copositive matrices, we refer the reader to [3], [26], and [20]. In Section 3, we examine the properties of the copositive range and show that it is a

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convex subset of the numerical range, that is, an interval whose endpoints are identified. In Section 4, we connect our findings to the Pareto spectrum of a copositive matrix.

2. Preliminaries. Let n be a positive integer. For the remainder of this paper, the real, square matrices will be denoted by $M_n(\mathbb{R})$. Additionally, the following notation is used throughout:

- $\mathbb{R}^n_+$ is the *nonnegative orthant*, that is, the set of all vectors in $\mathbb{R}^n$ with nonnegative entries. We interchangeably write $x \in \mathbb{R}^n_+$ or $x \geq 0$. The topological *interior* of $\mathbb{R}^n_+$ consists of the vectors x all of whose entries are positive, for which we write $x \in \operatorname{int} \mathbb{R}^n_+$ or $x > 0$. We write $\mathbb{R}_+$ for the nonnegative real line $\mathbb{R}^1_+$.
- The *spectrum* of A (multiset of eigenvalues) is denoted by $\sigma(A)$ and $\rho(A) = \max\{|\lambda| : \lambda \in \sigma(A)\}$ is the *spectral radius* of A.
- Let $\langle n\rangle = \{1, 2, ..., n\}$. $A[\alpha, \beta]$ is the submatrix of A whose rows and columns are indexed by $\alpha, \beta \subseteq \langle n\rangle$, respectively. The elements of α and β are assumed to be in ascending order.
- For any nonempty $\alpha \subseteq \langle n\rangle$, $A[\alpha] = A[\alpha, \alpha]$ is called a *principal submatrix* of A.

Definition 2.1. Let $A \in M_n(\mathbb{R})$ be a symmetric matrix. Then A is called *copositive* if $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n_+$. A is called *strictly copositive* if $x^T Ax > 0$ for all $x \in \mathbb{R}^n_+ \setminus \{0\}$.

The concept of copositivity was first introduced by Theodore S. Motzkin in 1952 [24], as a generalization of positive semidefiniteness. Therefore, the two matrix classes are analogous in many ways. The concept of copositivity was established in the early 1960s through the contributions of Baumert, Diananda, Hall and Newman, and Motzkin (resp., [1], [2], [8], [15], and [24]).

In optimization theory, copositive matrices play a role in offering a unified way for reformulating nonconvex mixed quadratic programs into convex programs [5]. Copositive matrices are also inherently of interest in the Linear Complementarity Problem (LCP) [6].

In differential equations, copositive matrices have applications in quadratic differential equations [13]. Copositivity is also used to model discrete markets and games in theoretical economics [11].

It is well known, that the set of copositive matrices form a proper cone in $M_n(\mathbb{R})$. Recall that a cone in a vector space is a subset K such that $a\,K \subseteq K$ for all $a \geq 0$. In addition, a cone K is said to be a *proper cone* if it is a closed, convex set that has a nonempty interior and is pointed (i.e., $K \cap (-K) = \{0\}$).

3. The copositive range. The concept of the copositive range of a copositive matrix, introduced below, is motivated by and is a natural extension of the numerical range of a matrix that is recalled next.

Definition 3.1. The numerical range (also known as the field of values) of $A \in \mathbf{M}_n(\mathbb{C})$ is the set

$$W(A) = \{x^* Ax \,:\, x \in \mathbb{C}^n,\, \|x\|_2 = 1\}.$$

When $A \in \mathbf{M}_n(\mathbb{R})$ is symmetric, its numerical range is an interval on the real line, namely,

$$W(A) = [\lambda_{\min}, \lambda_{\max}],$$

where $\lambda_{\min}$ and $\lambda_{\max}$ are the smallest and largest eigenvalues of A, respectively.

Next, we define the copositive range of a copositive matrix A.

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Definition 3.2. Let $A \in \mathbf{M}_n(\mathbb{R})$ be a copositive matrix. The *copositive range* of A is the set

$$CR(A) = \{x^T A x \,:\, x \in \mathbb{R}^n_+,\, \|x\|_2 = 1\}.$$

The numerical range of a matrix A is a well-studied set that captures information about A as a linear transformation, as well as the eigenvalues of A. The celebrated Toeplitz–Hausdorff Theorem states that $W(A)$ is a convex set (see [7], [9], [19], [23], including the original proof by Hausdorff [16]). We shall relate this result to the convexity of the copositive range. We direct the reader to [19, Chapter 1] for a comprehensive study of the numerical range.

3.1. Basic properties of the copositive range. In this section, we extend and itemize basic properties of the numerical range to the copositive range, establishing analogous results, and more:

(1) For any copositive $A \in M_n(\mathbb{R})$ and for any $a, b \in \mathbb{R}_+$, $a\,A + b\,I$ is copositive and

$$CR(a\,A + b\,I_n) = a\,CR(A) + b.$$

Proof. If $x \in \mathbb{R}^n_+$, where $\|x\|_2 = x^T x = 1$, then

$$x^T(a\,A + b\,I_n)x = ax^T Ax + bx^T x \in a\,CR(A) + b,$$ □

that is, $CR(a\,A + b\,I_n) \subseteq a\,CR(A) + b$. For the reverse inclusion, notice that

$$ax^T Ax + b = ax^T Ax + bx^T x = x^T(a\,A + b\,I_n)x.$$

(2) For any copositive matrices $A, B \in M_n(\mathbb{R})$,

$$CR(A + B) \subseteq CR(A) + CR(B).$$

Proof. Notice that

$$CR(A+B) = \{x^T(A+B)x \,:\, x \in \mathbb{R}^n_+,\, \|x\|_2 = 1\} = \{x^T Ax + x^T Bx \,:\, x \in \mathbb{R}^n_+,\, \|x\|_2 = 1\}$$
$$\subseteq CR(A) + CR(B).$$

The following counterexample shows that the reverse inclusion in (2) does not hold in general.

Example 3.3. Let

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

Clearly A and B are copositive since for all $x \in \mathbb{R}^2_+$, $x^T Ax = x_1^2 \geq 0$ and $x^T Bx = x_2^2 \geq 0$. Then,

$$A + B = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Now notice that

$$CR(A+B) = \{x^T(A+B)x \,:\, x \in \mathbb{R}^2_+,\, \|x\|_2 = 1\} = \{x^T x \,:\, x \in \mathbb{R}^2_+,\, \|x\|_2 = 1\} = \{1\}.$$

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However, writing $x = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T \in \mathbb{R}$, we have

$$CR(A) = \{x^T Ax \,:\, x \in \mathbb{R}^2_+,\, \|x\|_2 = 1\} = \{x_1^2 \,:\, \|x\| = 1\} = [0, 1]$$

$$CR(B) = \{x^T Bx \,:\, x \in \mathbb{R}^2_+,\, \|x\|_2 = 1\} = \{x_2^2 \,:,\, \|x\| = 1\} = [0, 1];$$

thus $CR(A) + CR(B) = [0, 2]$ and so $CR(A) + CR(B) \not\subseteq CR(A + B)$.

(3) Clearly, when $A \in M_n(\mathbb{R})$ is copositive and thus symmetric, we have

$$CR(A^T) = CR(A).$$

(4) For any copositive $A \in M_n(\mathbb{R})$ and any principal submatrix $A[\alpha]$ of A, where $\alpha \subseteq \langle n\rangle$, $A[\alpha]$ is also copositive and

$$CR(A[\alpha]) \subseteq CR(A).$$

Proof. Without loss of generality, let $\alpha = \{1, 2, \dots, k\}$ $(k \le n)$; otherwise work with a permutation similarity of A. Let $x = \begin{bmatrix} w \\ 0 \end{bmatrix}$, where $w \in \mathbb{R}^k_+$. Then, with $A_{11} = A[\alpha]$ we have

$$w^T A_{11} w = \begin{bmatrix} w^T & 0 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} w \\ 0 \end{bmatrix} = x^T Ax \in CR(A).$$

Hence, $CR(A_{11}) \subseteq CR(A)$. ◻

(5) For any copositive $A \in M_n(\mathbb{R})$ and copositive $B \in M_m(\mathbb{R})$,

$$\text{convex hull}\, \{CR(A) \cup CR(B)\} = CR(A \oplus B).$$

Proof. First recall that $A \oplus B$ is the direct sum of A and B defined as

$$A \oplus B = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix} \in M_{m+n}(\mathbb{R}).$$

Given

$$CR(A) = \{x^T Ax \,:\, x \in \mathbb{R}^m_+,\, \|x\|_2 = 1\}$$
$$CR(B) = \{y^T By \,:\, y \in \mathbb{R}^n_+,\, \|y\|_2 = 1\},$$

the convex hull$\{CR(A) \cup CR(B)\}$ consists of all elements of the form

$$\mu a + (1 - \mu)b, \quad \text{where}\, \mu \in [0, 1], \quad a \in CR(A), \quad b \in CR(B).$$

Let

$$z = \begin{bmatrix} \sqrt{\mu}x \\ \sqrt{1 - \mu}y \end{bmatrix} \in \mathbb{R}^{m+n},$$

such that

$$\|z\|_2^2 = \|\sqrt{\mu}x\|_2^2 + \|\sqrt{1 - \mu}y\|_2^2 = \mu\|x\|_2^2 + (1 - \mu)\|y\|_2^2 = \mu + (1 - \mu) = 1. \tag{3.1}$$

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It follows that

$$z^T(A \oplus B)z = \begin{bmatrix} \sqrt{\mu}x^T & \sqrt{1-\mu}y^T \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix} \begin{bmatrix} \sqrt{\mu}x \\ \sqrt{1-\mu}y \end{bmatrix}, \tag{3.2}$$

$$= \mu x^T Ax + (1-\mu)y^T By, \tag{3.3}$$

$$= \mu a + (1-\mu)b, \tag{3.4}$$

showing that any convex combination of elements from $CR(A)$ and $CR(B)$ belongs to $CR(A \oplus B)$; that is, convex hull$\{CR(A) \cup CR(B)\} \subseteq CR(A \oplus B)$.
For the reverse inclusion, consider

$$CR(A \oplus B) = \{z^T(A \oplus B)z \,:\, z \in \mathbb{R}_+^{m+n},\, \|z\|_2 = 1\},$$

where $z = \begin{bmatrix} x \\ y \end{bmatrix}$ and $x \in \mathbb{R}_+^m$ and $y \in \mathbb{R}_+^n$. Then $\|z\|_2^2 = \|x\|_2^2 + \|y\|_2^2 = 1$ and

$$z^T(A \oplus B)z = x^T Ax + y^T By.$$

To show that any every element of $CR(A \oplus B)$ can be written as a convex combination of elements in $CR(A) \cup CR(B)$, we need to consider different cases. First assume $y = 0$, which implies $\|x\|_2^2 = \|x\|_2 = 1$. Then,

$$z^T(A \oplus B)z = x^T Ax \in CR(A).$$

Similarly, if $x = 0$, then $\|y\|_2 = 1$ and

$$z^T(A \oplus B)z = y^T By \in CR(B).$$

Now consider the case where x and y are both nonzero. Let $\|x\|_2 = \sqrt{\alpha}$ and $\|y\|_2 = \sqrt{1-\alpha}$ for some $\alpha \in [0,1]$. Next, let

$$\hat{x} = \frac{x}{\sqrt{\alpha}} \quad \text{and} \quad \hat{y} = \frac{y}{\sqrt{1-\alpha}},$$

to ensure that $\|\hat{x}\|_2 = \|\hat{y}\|_2 = 1$. It follows that

$$x^T Ax = \alpha \hat{x}^T A\hat{x} \quad \text{and} \quad y^T By = (1-\alpha)\hat{y}^T B\hat{y},$$

which implies

$$z^T(A \oplus B)z = x^T Ax + y^T By = \alpha \hat{x}^T A\hat{x} + (1-\alpha)\hat{y}^T B\hat{y}.$$

In all three cases, we have $CR(A \oplus B) \subseteq$ convex hull$\{CR(A) \cup CR(B)\}$. Thus by both inclusions, convex hull$\{CR(A) \cup CR(B)\} = CR(A \oplus B)$. □

(6) Given a symmetric $A \in M_n(\mathbb{R})$ and a permutation matrix P, $CR(A) = CR(PAP^T)$.

Proof. Let $x \in \mathbb{R}_+^n$ such that $\|x\|_2 = 1$ and define $y = Px$. Since P is a permutation matrix, we know that $y \in \mathbb{R}_+^n$. Additionally, P is orthogonal which implies that it preserves the Euclidean norm. Hence,

$$\|y\|_2 = \|Px\|_2 = \|x\|_2 = 1.$$

It follows that

$$x^T Ax = (P^T y)^T A(P^T y) = y^T(PAP^T)y \in CR(PAP^T),$$

and $CR(A) \subseteq CR(PAP^T)$.

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Now for $x \in \mathbb{R}^n_+$ and $\|x\|_2 = 1$, let $z = P^T x$. Then $\|z\|_2 = \|P^T x\|_2 = \|x\|_2 = 1$ and

$$x^T(PAP^T)x = (P^T x)^T A(P^T x) = z^T Az \in CR(A).$$

Thus by double inclusion, $CR(A) = CR(PAP^T)$. ∎

(7) The numerical range of any matrix is known to contain the spectrum of A, $\sigma(A)$. Moreover, if A is a normal matrix (e.g., symmetric), then $W(A)$ is the convex hull of the eigenvalues of A. Neither of these results is generally true for $CR(A)$. Indeed, consider the matrix in Example 3.6 forward. Note that $\sigma(A) = \{-\sqrt{6}, \sqrt{6}, 4\}$, but $CR(A) = [\ell, 4]$ for some $\ell > 0$. So $\lambda = -\sqrt{6} \notin CR(A)$ and thus convex hull$\{\sigma(A)\} \neq CR(A)$.
A weak version of (7) holds for copositive matrices as seen next.

(8) Let $A \in M_n(\mathbb{R})$ be copositive. Then its spectral radius $\rho(A)$ is an eigenvalue of A; see [17]. The corresponding eigenspace of $\rho(A)$ may not contain a nonnegative eigenvector x and thus $\rho(A)$ may not belong to $CR(A)$; see [4]. However, [4, Theorem 1] provides sufficient conditions for $\rho(A) \in CR(A)$.

3.2. Convexity of the copositive range. The copositive range can indeed be viewed as a domain-restricted version of the numerical range. Indeed, in $W(A)$ we have that the unit vectors $x \in \mathbb{C}^n$, while in $CR(A)$, $x \in \mathbb{R}^n_+$

The convexity of domain-restricted numerical ranges has been systematically studied by Feldman et al. in [10] and also considered in [12]. Domain restrictions of the numerical range are not necessarily convex. However, as the next theorem shows, $CR(A)$ is convex set.

THEOREM 3.4. *Let $A \in \mathbf{M}_n(\mathbb{R})$ be copositive. Then $CR(A)$ is convex subset of $W(A)$.*

Proof. Consider two elements of $CR(A)$, $\alpha = x^T Ax, \beta = y^T Ay$, with $\alpha \leq \beta$, where $x = [x_j] \geq 0, y = [y_j] \geq 0, \|x\|_2 = \|y\|_2 = 1$. For each $t \in [0, 1]$ define the vector

$$u(t) = [u_j(t)], \quad u_j(t) = \sqrt{(1-t)x_j^2 + ty_j^2},\ j = 1, 2, \ldots n.$$

Clearly, $u(t) \geq 0$, $u(0) = x$, and $u(1) = y$. Also $\|u(t)\|_2 = 1$ because

$$u(t)^T u(t) = (1-t)\sum_{j=1}^n x_j^2 + t\sum_{j=1}^n y_j^2 = (1-t) + t = 1.$$

Therefore, $u(t) \in CR(A)$ for all $t \in [0, 1]$. Since

$$u^T(0)Au(0) = x^T Ax = \alpha,\ \ u^T(1)Au(1) = y^T Ay = \beta,$$

it follows by continuity of the quadratic form that

$$[\alpha, \beta] = \{u^T(t)Au(t)\ :\ t \in [0, 1]\} \subseteq CR(A).$$

We conclude that $CR(A)$ is a convex subset of $W(A)$. ∎

COROLLARY 3.5. *For copositive $A \in \mathbf{M}_n(\mathbb{R})$, $CR(A)$ is a closed interval in $W(A) \cap \mathbb{R}_+$.*

Proof. Let K be the intersection of the surface of the unit sphere in $\mathbb{C}^n$ with $\mathbb{R}^n_+$. Since K is a compact set (closed and bounded), the continuous map $x \to x^*Ax$ (a map $K \to \mathbb{R}$) maps K to a closed set. Thus, $CR(A)$ is a closed subset of $\mathbb{R}_+$. It follows by Theorem 3.4 that $CR(A)$ is a closed, convex subset of the closed interval $W(A)$. Thus, $CR(A)$ must be a closed subinterval of $W(A) \cap \mathbb{R}_+$. ∎

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As aforementioned, when A is symmetric, $W(A) = [\lambda_{min}, \lambda_{max}]$, where λ_{min} and λ_{max} are the smallest and largest eigenvalue of A, respectively. By Corollary 3.5, when A is copositive, there exist $\ell \geq \lambda_{min}$ and $r \leq \lambda_{max}$ such that

$$CR(A) = [\ell, r] \subseteq W(A) \cap \mathbb{R}_+.$$

It is our aim next to specify the endpoints of $CR(A) = [\ell, r]$.

First, let us observe in the next example that it is not necessarily the case that $CR(A) = W(A) \cap \mathbb{R}_+$.

Example 3.6. Consider the copositive matrix

$$A = \begin{bmatrix} 1 & 3 & -1 \\ 3 & 1 & 1 \\ -1 & 1 & 2 \end{bmatrix}.$$

The spectrum of A is $\sigma(A) = \{-\sqrt{6}, \sqrt{6}, 4\}$ so that $CR(A) = [\ell, r] \subseteq W(A) = [-\sqrt{6}, 4]$. Then $W(A) \cap \mathbb{R}_+ = [0, 4]$. The endpoint $4 \in CR(A)$ because the eigenvalue 4 corresponds to a nonnegative eigenvector of A. However, the endpoint $0 \notin CR(A)$ because

$$x^T A x \neq 0 \quad \text{for all nonzero } x = [x_1\ x_2\ x_3]^T \in \mathbb{R}^3_+.$$

Indeed, it can be verified that for all nonzero $x \in \mathbb{R}^3_+$,

$$x^T A x = (x_1 - x_3)^2 + x_2^2 + x_3^2 + 6x_1x_2 + 2x_2x_3 > 0.$$

As a consequence, $CR(A) = [\ell, 4]$ for some $\ell > 0$.

Formally, it is clear that the extreme points of $CR(A) = [\ell, r]$ are indeed the solutions of the following constraint optimization problems:

$$\ell = \min_{x \neq 0} \frac{x^T A x}{x^T x} \qquad r = \max_{x \neq 0} \frac{x^T A x}{x^T x} \tag{3.5}$$
$$\text{subject to } x \geq 0 \qquad \text{subject to } x \geq 0.$$

Recall the fundamental relation between the copositive range of a copositive matrix A and its submatrices: By Property (4) in Section 3.1, we have that for each nonempty $\alpha \subseteq \langle n \rangle$, $A[\alpha]$ is copositive and

$$CR(A[\alpha]) \subseteq CR(A).$$

As a consequence we have the following result, which hints at the main result stated in Theorem 3.8.

Proposition 3.7. *Let $A \in M_n(\mathbb{R})$ be copositive, where $CR(A) = [\ell, r]$ and $CR(A[\alpha]) = [\ell_\alpha, r_\alpha]$. Then*

$$\ell \leq \ell_\alpha \quad \text{and} \quad r_\alpha \leq r.$$

We proceed to solve the constraint optimization problems in (3.5). To minimize $f(x) = x^T A x$ subject to the constraint $x \geq 0$ and $x^T x = 1$, we can apply the Karush–Kuhn–Tucker (KKT) conditions. The problem is a quadratic form with equality and inequality constraints, and the KKT conditions provide a way to handle both types of constraints.

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THEOREM 3.8. *Let $A \in M_n(\mathbb{R})$ be a symmetric copositive matrix and $CR(A) = [\ell, r]$ be the copositive range of A. Denoting $\langle n \rangle = \{1, 2, \ldots, n\}$, we have*

$$\ell = \min_{\alpha \subseteq \langle n \rangle} \min \{\lambda \in \sigma(A[\alpha]) : A[\alpha]x = \lambda x,\, x \in \mathbb{R}_+^{|\alpha|} \setminus \{0\}\}, \text{ and}$$

$$r = \max_{\alpha \subseteq \langle n \rangle} \max \{\lambda \in \sigma(A[\alpha]) : A[\alpha]x = \lambda x,\, x \in \mathbb{R}_+^{|\alpha|} \setminus \{0\}\}.$$

Proof. We will begin by applying the KKT conditions to minimize

$$f(x) = x^T A x,$$

subject to:

$$g(x) = x^T x - 1 = 0 \quad \text{(equality constraint)},$$
$$x \geq 0 \text{ i.e., for each } i,\ x_i \geq 0 \quad \text{(inequality constraints)}.$$

The Lagrangian function is

$$\mathcal{L}(x, \lambda, \mu) = x^T A x - \lambda(x^T x - 1) - \sum_{i=1}^{n} \mu_i x_i,$$

where

- λ is the Lagrange multiplier for the equality constraint,
- $\mu = [\mu_1, \mu_2, \ldots, \mu_n]^T$ comprises the Lagrange multipliers for the inequality constraints.

The KKT conditions state that the optimal solution to the minimization problem must satisfy the following:

1. Stationarity: The gradient of the Lagrangian function is:

$$\nabla_x \mathcal{L}(x, \lambda, \mu) = \nabla_x (x^T A x) - \lambda \nabla_x [(x^T x - 1)] - \nabla_x \left(\sum_i \mu_i x_i \right). \tag{3.6}$$

Since A is symmetric,

$$\nabla_x (x^T A x) = (A + A^T)x = 2Ax,$$

and

$$\nabla_x (x^T x - 1) = \nabla_x \left(\sum_i x_i^2 - 1 \right) = 2x,$$

$$\nabla_x \left(\sum_i \mu_i x_i \right) = \mu.$$

For the stationarity condition, the gradient of the Lagrangian with respect to x must be set to zero. Combining the three terms from above we have

$$\nabla_x \mathcal{L}(x, \lambda, \mu) = 2Ax - 2\lambda x - \mu = 0, \tag{3.7}$$

which simplifies to $2(Ax - \lambda x) = \mu$, or equivalently,

$$Ax = \lambda x + \frac{1}{2}\mu. \tag{3.8}$$

Note that this implies that x satisfies an eigenvector-like equation for A, perturbed by a multiple of the nonnegativity constraint vector, μ.

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2. Primal feasibility: The original inequality and equality constraints
$$x \geq 0 \quad \text{and} \quad x^T x = 1,$$
must hold.
3. Dual feasibility: The Lagrange multipliers associated with the nonnegativity constraint must be nonnegative.
4. Complementary slackness: For each i,
$$\mu_i x_i = 0;$$
that is, if $x_i > 0$, then $\mu_i = 0$, and if $\mu_i > 0$, then $x_i = 0$.

Now note that each feasible solution x lies in a subspace defined by the support of x, namely, the set of indices i, where $x_i > 0$. Let $S \subseteq \{1, 2, \ldots, n\}$ represent the support of x. Since x_i being nonzero implies $\mu_i = 0$, equation (3.8) in the stationarity condition becomes $A[S]\, x[S] = \hat{\lambda}\, x[S]$, where $\hat{\lambda}$ is an eigenvalue of $A[S]$.

Thus, for a given support set S, if $A[S]$ has an eigenvalue with a corresponding nonnegative eigenvector $x[S]$ and $x[S]^T x[S] = 1$. Hence, $x[S]$ is feasible for the original constraints $x \geq 0$ and $x^T x = 1$. This implies that
$$x[S]^T\, A[S]\, x[S] = \hat{\lambda},$$
and $\hat{\lambda}$ is a candidate value $x^T A x$ in the original minimization problem.

It follows that ℓ, the minimum value of $x^T A x$ over $x \geq 0$ with $x^T x = 1$, is the smallest among the eigenvalues of the principal submatrices of A with corresponding nonnegative eigenvectors, that is,
$$\ell = \min_{\alpha \subseteq \langle n \rangle} \min \{\lambda \in \sigma(A[\alpha]) \,:\, A[\alpha]x = \lambda x,\, x \in \mathbb{R}_+^{|\alpha|} \setminus \{0\}\}.$$

The case of the maximum value of $x^T A x$ over $x \geq 0$ with $x^T x = 1$ can be treated similarly and be characterized as the largest among the eigenvalues of the principal submatrices of A with corresponding nonnegative eigenvectors, that is,
$$r = \max_{\alpha \subseteq \langle n \rangle} \max \{\lambda \in \sigma(A[\alpha]) \,:\, A[\alpha]x = \lambda x,\, x \in \mathbb{R}_+^{|\alpha|} \setminus \{0\}\}.$$
□

Remark 3.9. While KKT as used in the theorem above serves as a theoretical framework by providing necessary conditions for a optimal solution to a constrained optimization problem, Sequential Least Squares Programming (SLSQP) is a more suitable algorithm that numerically solves the problem of finding the endpoints of the copositive range. By utilizing the gradient of the objective function $f(x)$ and the constraints, SLSQP iteratively searches for an optimal solution that satisfies the KKT conditions at convergence. The application of SLSQP is illustrated next.

Example 3.10. We consider the matrix A from Example 3.6, for which we found that its copositive range is $CR(A) = [\ell, 4]$ with $\ell > 0$. We shall apply the KKT conditions and SLSQP to compute ℓ and verify that it corresponds to the smallest eigenvalue of a principal submatrix. We have
$$A = \begin{bmatrix} 1 & 3 & -1 \\ 3 & 1 & 1 \\ -1 & 1 & 2 \end{bmatrix}.$$

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The optimization problem is given by:

$$\min_x x^T A x,$$

subject to $x \geq 0$ and $x^T x = 1$.

For the vector $x_0 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ as an initial guess, SLSQP yields the following output:

- Optimal value: 0.38196...
- Optimal vector $x = \begin{bmatrix} 0.85065... & 0 & 0.525731... \end{bmatrix}^T$

Indeed, the support of x is $S = \{1, 3\}$, corresponding to the principal submatrix of A,

$$A[S] = \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix},$$

which has an eigenvalue $\hat{\lambda} = 0.38196...$ with $\begin{bmatrix} 0.85065... & 0.525731... \end{bmatrix}^T$ as the corresponding eigenvector.

The following examples offer additional validation of the evaluation of $CR(A) = [\ell, r]$.

Example 3.11. Consider the copositive matrix

$$A = \begin{bmatrix} 1 & 1 & -1 \\ 1 & 2 & 0 \\ -1 & 0 & 5 \end{bmatrix}. \tag{3.9}$$

SLSQP output:

- $\hat{\lambda}_{\min} = 0.763932, \qquad \begin{bmatrix} 0.9732 & 0 & 0.2298 \end{bmatrix}^T$
- $\hat{\lambda}_{\max} = 5, \qquad \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}^T$

Corresponding principal submatrices of A:

- $A[\{1, 3\}] = \begin{bmatrix} 1 & -1 \\ -1 & 5 \end{bmatrix}$ with a minimum eigenvalue 0.763932 and the corresponding eigenvector $\begin{bmatrix} 0.973249 & 0.229753 \end{bmatrix}^T$
- $A[\{3, 3\}] = \begin{bmatrix} 5 \end{bmatrix}$ with an eigenvalue of 5 and the corresponding eigenvector of $\begin{bmatrix} 0 & 0 & 1 \end{bmatrix}^T$

Thus, $CR(A) = [0.763932, 5]$.

Example 3.12. Consider the copositive matrix

$$A = \begin{bmatrix} 13 & -9 & 28 \\ -9 & 12 & -11 \\ 28 & -11 & 20 \end{bmatrix}. \tag{3.10}$$

SLSQP output:

- $\hat{\lambda}_{\min} = 3.4862, \qquad \begin{bmatrix} 0.6872 & 0.7265 & 0 \end{bmatrix}^T$
- $\hat{\lambda}_{\max} = 44.717902, \qquad \begin{bmatrix} 0.6618 & 0 & 0.7497 \end{bmatrix}^T$

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Corresponding principal submatrices of A:

- $A[\{1,2\}] = \begin{bmatrix} 13 & -9 \\ -9 & 12 \end{bmatrix}$ with a minimum eigenvalue 3.48612 and the corresponding eigenvector $\begin{bmatrix} 0.6872 & 0.7265 \end{bmatrix}^T$
- $A[\{1,3\}] = \begin{bmatrix} 13 & 28 \\ 28 & 20 \end{bmatrix}$ with eigenvalue 44.717902 and corresponding eigenvector $\begin{bmatrix} 0.6618 & 0.7497 \end{bmatrix}^T$

Thus, $CR(A) = [3.4862, 44.717902]$.

Example 3.13. In this example, we observe that the copositive range, unlike the numerical range, is not necessarily invariant under (real) unitary similarity, primarily because for unitary $Q \in M_n(\mathbb{R})$ (i.e., real orthogonal Q), Q^TAQ is not necessarily copositive. Furthermore, even if Q^TAQ happens to be copositive, $CR(A)$ and $CR(Q^TAQ)$ may still differ; both instances are illustrated by simple matrices next. Let

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \text{and} \quad Q = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$

so that A is copositive and Q is real unitary. Then

$$Q^TAQ = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix},$$

which is clearly not copositive. Now let

$$B = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix},$$

be another copositive matrix. Then

$$Q^TBQ = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix},$$

which is copositive. However, $CR(B) = [2,3] \neq [1,2] = CR(Q^TBQ)$.

4. Relation to Pareto Eigenvalues.

As aforementioned, detecting copositive matrices presents a significant challenge. Even if all the eigenvalues of a symmetric $A \in M_n(\mathbb{R})$ are known, this alone does not suffice to determine the copositivity of A. For example, if all the eigenvalues of A are nonnegative, then A is positive semidefinite and therefore copositive. However, the converse does not hold as not every copositive matrix is positive semidefinite.

Although the spectrum of A gives us some insight into the copositivity of A, what is more important to know about A is its Pareto spectrum, which consists of values associated with the cone-constrained minimization problem

$$\mu(A) = \min_{\substack{x \geq 0 \\ \|x\|=1}} x^TAx, \tag{4.11}$$

Writing down the optimality conditions for (4.11), we have

$$x \geq 0, \quad Ax - \lambda x \geq 0 \quad x^T(Ax - \lambda x) = 0, \tag{4.12}$$

$$\|x\| = 1, \tag{4.13}$$

where $\lambda \in \mathbb{R}$ is viewed as a Lagrange multiplier associated with the normalization constraint in (4.13).

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Definition 4.1. [25] 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 (4.12) 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.

It is known that for a given matrix $A \in M_n(\mathbb{R})$, every Pareto eigenvalue of A comes from some principal submatrix of A where the corresponding eigenvector is nonnegative. For copositive matrix $A \in M_n(\mathbb{R})$ and nonzero $x \in \mathbb{R}^n_+$, it follows that

$$x^T(Ax - \lambda x) = 0 \implies x^T Ax = \lambda x^T x \implies \lambda = \frac{x^T Ax}{x^T x} \geq 0.$$

The link between Pareto spectra and copositivity is provided in the following theorem.

Theorem 4.2. [18] *A symmetric matrix A of order n is copositive if and only if all the Pareto eigenvalues of A are nonnegative.*

The key observation for this theorem is that since A is symmetric, $\mu(A)$ turns out to be the smallest element of $\Pi(A)$. That is,

$$\mu(A) = \min_{\substack{x\geq 0 \\ \|x\|=1}} x^T Ax = \min_{\lambda\in\Pi(A)} \lambda.$$

For more information on computing Pareto spectra, we refer the readers to [18] and [25].

To connect Pareto spectra of copositive matrices to the copositive range as introduced herein, we recall the following result by Kaplan ([21], [22]).

Proposition 4.3. *A symmetric matrix A of order n is copositive if and only if*

$$A[S]\xi = \lambda\xi \quad \textit{and} \quad \xi \in \operatorname{int}(\mathbb{R}^{|S|}_+) \implies \lambda \geq 0,$$

for every nonempty index set $S \subseteq \{1, 2, \ldots, n\}$.

We know from Property (4) in Section 3.1 that every principal submatrix of copositive $A \in M_n(\mathbb{R})$ is also copositive. Combining Proposition 4.3 and Property (4) of $CR(A)$, it follows that the Pareto spectrum of a copositive matrix A contains all nonnegative Pareto eigenvalues of the principal submatrices of A that admit nonzero nonnegative eigenvectors. This allows us to conclude the following.

Proposition 4.4. *Let $A \in \mathbf{M}_n(\mathbb{R})$ be a copositive matrix with copositive range $[\ell, r]$ and Pareto spectrum $\Pi(A)$. Then $\ell = \min_{\lambda\in\Pi(A)} \lambda$ and $r = \max_{\lambda\in\Pi(A)} \lambda$.*

Consider the following illustrative example.

Example 4.5. Consider the copositive matrix $A = \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix}$, with $\sigma(A) = \{0.38197, 2.6180\}$, so that A is copositive. The Pareto spectrum of A is $\Pi(A) = \{0.38197,\ 1,\ 2\}$; indeed

$$\min_{\substack{x\geq 0 \\ \|x\|=1}} x^T Ax = 0.38197 \quad \text{and} \quad \max_{\substack{x\geq 0 \\ \|x\|=1}} x^T Ax = 2.$$

Thus, $CR(A) = [0.38197, 2]$.

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REMARK 4.6. We conclude by recalling a result on the numerical range and posing a related question about the copositive range. Let $GL_n(\mathbb{C})$ denote the set of all invertible matrices in $\mathbf{M}_n(\mathbb{C})$. It is known (Hildebrandt's Theorem) that for any $A \in \mathbf{M}_n(\mathbb{C})$,

$$\bigcap_{S \in GL_n(\mathbb{C})} W(S^{-1}AS) = \text{convex hull}\{\sigma(A)\}. \tag{4.14}$$

Copositivity is not preserved under similarity. It is, however, preserved under congruence by nonsingular nonnegative monomial matrices (i.e., matrices M having exactly one positive element in each row and column). Let us denote this group of matrices M by $\mathcal{F}_n \subset GL_n(\mathbb{C})$. Given a copositive matrix $A \in \mathbf{M}_n(\mathbb{R})$, we ask whether or not there is a result analogous to (4.14) involving the Pareto spectrum of A and the set

$$\bigcap_{M \in \mathcal{F}_n} CR(M^T AM).$$

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