# The extreme rays of the $5 \times 5$ copositive cone

Roland Hildebrand *

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### Abstract

We give an explicit characterization of all extreme rays of the cone $\mathcal{C}_5$ of $5 \times 5$ copositive matrices. The results are based on the work of Baumert [L. D. Baumert, "Extreme copositive quadratic forms", PhD thesis, 1965], where an implicit characterization was given. We show that the class of extreme rays found by Baumert forms a 10-dimensional variety, which can be parameterized in a semi-trigonometric way.

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## 1 Introduction

A real symmetric $n \times n$ matrix $A$ is called *copositive* if $x^T A x \geq 0$ for all $x \in \mathbb{R}^n_+$. The set of copositive matrices forms a convex cone $\mathcal{C}_n$, the *copositive cone*. Clearly $A$ is copositive if it is either positive semi-definite or if all its elements are nonnegative. Hence both the cone $S_+(n)$ of all $n \times n$ real symmetric positive semi-definite matrices and the cone $NN_n$ of all $n \times n$ real symmetric nonnegative matrices are contained in $\mathcal{C}_n$. It is a classical result by Diananda [5] that for $n \leq 4$ the cone $\mathcal{C}_n$ equals the sum $S_+(n) + NN_n$. For $n \geq 5$ there exist matrices in $\mathcal{C}_n$ which cannot be represented as a sum of a positive semi-definite matrix and a nonnegative matrix. An example of such a matrix is the *Horn form* [6]

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

While the sum $S_+(n) + NN_n$ can easily be handled algorithmically, problems involving the copositive cone are in general difficult. Of particular help in the description of the copositive cone is any information on its extreme rays. Since deciding inclusion of an integer matrix into the copositive cone is NP-complete [8], a general explicit characterization of the extreme rays of $\mathcal{C}_n$ is unlikely to be found. However, those extreme rays which belong to the sum $S_+(n) + NN_n$ have been characterized completely, and the Horn form (1) has been characterized as an extreme ray of $\mathcal{C}_5$ which does not belong to this sum [6]. Baumert [3] has shown that any other extreme ray of $\mathcal{C}_5$ must be a solution of a certain system of algebraic equations, and has provided an explicit example, see also the publications [1], [2]. In [3], a procedure is also presented how to construct an extreme ray of $\mathcal{C}_{n+1}$ from an extreme ray of $\mathcal{C}_n$. Those extreme rays with elements only from the set $\{-1, 0, +1\}$ have been characterized in [7].

Much work has also been devoted to characterize the difference between the completely positive cone $\mathcal{C}_n^*$ and the intersection $S_+(n) \cap NN_n$, which are the dual cones to $\mathcal{C}_n$ and $S_+(n) + NN_n$, respectively. Special emphasis has been made on the $5 \times 5$ case. An earlier paper with a partial characterization of the $5 \times 5$ completely positive cone is [9]. In [4] extreme rays of $S_+(5) \cap NN_5$ which do not belong to $\mathcal{C}_5^*$ are characterized and it is shown how to separate them from $\mathcal{C}_5^*$ by a copositive matrix.

In this note, we complete Baumerts characterization [3] of the extreme rays of the cone $\mathcal{C}_5$ by providing an exhaustive explicit description. The key step to solving Baumerts algebraic system of equations will be a trigonometric parametrization of these solutions, which yields also a simple semi-trigonometric parametrization of the generic extreme ray of $\mathcal{C}_5$.

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*LJK, Université Grenoble 1 / CNRS, 51 rue des Mathématiques, BP53, 38041 Grenoble cedex, France (`roland.hildebrand@imag.fr`, tel. +33-476-635714, fax +33-476-631263).

## 1.1 Notations

For a given $n \geq 1$, denote by $e_{ij}$, $i,j = 1, \ldots, n$, the generators of the extreme rays of the cone $NN_n$, normalized such that their elements are from the set $\{0,1\}$. Let $e_i$, $i = 1, \ldots, n$ be the canonical basis vectors of $\mathbb{R}^n$, and let $\Delta_n = \{x \in \mathbb{R}^n_+ \mid \sum_{j=1}^n x_j = 1\}$ be their convex hull.

Let $\text{Aut}(\mathbb{R}^n_+)$ be the automorphism group of the positive orthant. It is generated by all $n \times n$ permutation matrices and by all $n \times n$ diagonal matrices with positive diagonal elements. This group generates a group $\mathcal{G}_n$ of automorphisms of $\mathcal{C}_n$ by $A \mapsto GAG^T$, $G \in \text{Aut}(\mathbb{R}^n_+)$.

For any nonzero $x \in \mathbb{R}^n_+$, the *pattern* of $x$ will be the vector $\text{sgn}(x)^T$, where the sign function is applied elementwise.

We will work a lot with systems of equations that can be obtained from each other by a cyclical shift of indices. To simplify notation, we introduce the following index convention. The notation $k(n)$ means that the index $k$, which can be any integer, has to be shifted modulo $n$ into the range $1, \ldots, n$. With this convention, e.g., $\varphi_{6(5)} := \varphi_1$.

Let $A$ be an $n \times n$ matrix, $v \in \mathbb{R}^n$ a vector, and $I \subset \{1, \ldots, n\}$ a subset of indices. By $A_I$ we denote the principal submatrix of $A$ whose elements have row and column indices in $I$, and by $v_I$ the subvector of $v$ whose elements have indices in $I$. In the case $n = 5$, we define the special index sets $I_j^4 = \{1, \ldots, n\} \setminus \{j\}$ and $I_j^3 = \{j - 1(5), j, j + 1(5)\}$, $j = 1, \ldots, 5$.

Finally, we define the 5-parametric family of matrices

$$T(\varphi) = \begin{pmatrix} 1 & \sin\varphi_4 & -\cos(\varphi_4 + \varphi_5) & -\cos(\varphi_2 + \varphi_3) & \sin\varphi_3 \\ \sin\varphi_4 & 1 & \sin\varphi_5 & -\cos(\varphi_5 + \varphi_1) & -\cos(\varphi_3 + \varphi_4) \\ -\cos(\varphi_4 + \varphi_5) & \sin\varphi_5 & 1 & \sin\varphi_1 & -\cos(\varphi_1 + \varphi_2) \\ -\cos(\varphi_2 + \varphi_3) & -\cos(\varphi_5 + \varphi_1) & \sin\varphi_1 & 1 & \sin\varphi_2 \\ \sin\varphi_3 & -\cos(\varphi_3 + \varphi_4) & -\cos(\varphi_1 + \varphi_2) & \sin\varphi_2 & 1 \end{pmatrix},$$

where $\varphi = (\varphi_1, \ldots, \varphi_5)^T$ is a quintuple of angles. In various settings in the paper, these angles will satisfy one or more of the inequalities

$$\varphi_j \;>\; -\frac{\pi}{2} \qquad \forall\, j = 1, \ldots, 5, \qquad (2)$$

$$\varphi_j + \varphi_{j+1(5)} \;<\; 0 \qquad \forall\, j = 1, \ldots, 5, \qquad (3)$$

$$\sum_{j=1}^5 \varphi_j \;<\; -\frac{3\pi}{2}, \qquad (4)$$

$$t_j = \sin(\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)}) - \cos(\varphi_{j-2(5)} + \varphi_{j+2(5)}) \;>\; 0, \qquad \forall\, j = 1, \ldots, 5. \qquad (5)$$

## 2 Known results

In this section we collect known results on the structure of the cone $\mathcal{C}_n$ and its extreme rays, in particular for the value $n = 5$, which will be used later.

**Theorem 2.1.** *[6, Theorem 3.2] The extreme rays of $\mathcal{C}_n$ which belong to $S_+(n) \cap NN_n$ are generated by $e_{ij}$, $i, j = 1, \ldots, n$, and by matrices of the form $aa^T$, where the vectors $a \in \mathbb{R}^n$ contain both positive and negative elements.*

For the following simple fact, we did not find an explicit reference in the literature, but believe it is widely known.

**Lemma 2.2.** *Let $A \in \mathcal{C}_n$ be a copositive matrix, and let $x \in \mathbb{R}^n_+$ be such that $x^T A x = 0$. Let further $I = \{i \in \{1, \ldots, n\} \mid x_i > 0\}$. Then $A_I$ is positive semi-definite.*

*Proof.* Under the assumptions of the lemma, the restriction of the quadratic form $A$ to the linear subspace spanned by $\{e_i \mid i \in I\}$ possesses the local minimum $x_I$. Hence this minimum is global, which implies $A_I \succeq 0$. $\qquad\square$

The following slight reformulation of [3, Theorem 4.3] will be the departure point for the proof of our main result.

**Theorem 2.3.** *Let $A \in \mathcal{C}_5$ generate an extreme ray, and suppose that $A$ is neither an element of the sum $S_+(5) + NN_5$ nor in the orbit of the Horn form (1) under the action of $\mathcal{G}_5$. Then there exists a permutation matrix $P$ such that the set $\{x \in \Delta_5 \,|\, x^T P^T A P x = 0\}$ consists of 5 isolated points with patterns $(11001), (11100), (01110), (00111), (10011)$.*

*Proof.* Since $A$ is an extreme copositive matrix not contained in $NN_5$, all its diagonal elements have to be positive [3, p.17]. Then there exists a diagonal matrix $D \in \operatorname{Aut}(\mathbb{R}_+^5)$ such that the diagonal elements of $DAD$ all equal 1. But $DAD$ is also an extreme copositive matrix, satisfying the same exclusion conditions as $A$. The assertion of the theorem for the product $DAD$ now follows from application of [3, Theorem 4.3] to this product. Finally note that if $x$ is a zero of the quadratic form $DAD$, then $Dx$ is a zero of $A$ with the same pattern, which yields the assertion of the theorem also for $A$. $\qquad\square$

# 3 Main result

In this section we prove the following result.

**Theorem 3.1.** *Let $A \in \mathcal{C}_5$ generate an extreme ray, and suppose that $A$ is neither an element of the sum $S_+(5) + NN_5$ nor in the orbit of the Horn form (1) under the action of $\mathcal{G}_5$. Then $A$ is of the form*

$$A = P \cdot D \cdot T(\varphi) \cdot D \cdot P^T, \tag{6}$$

*where $P$ is a permutation matrix, $D = \operatorname{diag}(d_1, d_2, d_3, d_4, d_5)$ with $d_j > 0$, $j = 1, \ldots, 5$, and the quintuple $\varphi$ is an element of the set*

$$\Phi = \{\varphi \in \mathbb{R}^5 \,|\, \varphi \text{ satisfies (2,4)}\}. \tag{7}$$

*Conversely, for every permutation matrix $P$, every diagonal matrix $D$ with positive diagonal entries, and every quintuple of angles $\varphi \in \Phi$, the matrix $A$ given by (6) generates an extreme ray of $\mathcal{C}_5$ with the above exclusion properties.*

We postpone the proof of the theorem and first provide the following technical lemmas.

**Lemma 3.2.** *Let $C \in S_+(3)$ be such that the set $\{x \in \Delta_3 \,|\, x^T C x = 0\}$ consists of an isolated point in the interior of $\Delta_3$. Then $C$ can be represented in the form*

$$C = D \begin{pmatrix} 1 & \sin \varphi_1 & -\cos(\varphi_1 + \varphi_2) \\ \sin \varphi_1 & 1 & \sin \varphi_2 \\ -\cos(\varphi_1 + \varphi_2) & \sin \varphi_2 & 1 \end{pmatrix} D, \tag{8}$$

*where $D = \operatorname{diag}(d_1, d_2, d_3)$ with $d_j > 0$, $j = 1, 2, 3$, and $\varphi_1, \varphi_2$ satisfy the inequalities*

$$\varphi_j > -\frac{\pi}{2}, \qquad j = 1, 2, \tag{9}$$

$$\varphi_1 + \varphi_2 < 0. \tag{10}$$

*Conversely, for every matrix $D = \operatorname{diag}(d_1, d_2, d_3)$ with $d_j > 0$, $j = 1, 2, 3$, and angles $\varphi_1, \varphi_2$ satisfying (9,10) the matrix $C$ given by (8) is in $S_+(3)$ and the set $\{x \in \Delta_3 \,|\, x^T C x = 0\}$ consists of an isolated point in the interior of $\Delta_3$, which is proportional to $D^{-1}(\cos \varphi_2, -\sin(\varphi_1 + \varphi_2), \cos \varphi_1)^T$.*

*Proof.* Assume the conditions of the first part of the lemma. If $C$ has a zero diagonal entry, say $C_{11} = 0$, then $e_1^T C e_1 = 0$, which leads to a contradiction with the assumption that the zero of $C$ is in the interior of $\Delta_3$. Hence the diagonal elements of $C$ are positive. Put $d_j = \sqrt{C_{jj}}$, $j = 1, 2, 3$, and $D = \operatorname{diag}(d_1, d_2, d_3)$. If an off-diagonal element of $C' = D^{-1} C D^{-1}$ equals $-1$, say $C'_{12}$, then $(e_1 + e_2)^T C'(e_1 + e_2) = 0$, and $D^{-1}(e_1 + e_2)$ is a zero of $C$ in $\partial \Delta_3$, again leading to a contradiction. Therefore the off-diagonal elements of $C'$ are in the interval $(-1, 1]$, and we find angles $\varphi_1, \varphi_2 \in (-\frac{\pi}{2}, \frac{\pi}{2}]$ (and hence satisfying (9)) such that $C'_{12} = \sin \varphi_1$, $C'_{23} = \sin \varphi_2$. We then have

$$\det C' = 1 + 2C'_{13} \sin \varphi_1 \sin \varphi_2 - \sin^2 \varphi_1 - \sin^2 \varphi_2 - (C'_{13})^2 = 0,$$

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which yields $C'_{13} = \sin\varphi_1 \sin\varphi_2 + \sigma\cos\varphi_1\cos\varphi_2$, where $\sigma = \pm 1$. If $C'$ is of rank 1, then $\varphi_1 = \varphi_2 = \frac{\pi}{2}$ and hence $C'$ is the all-ones matrix, which contradicts the presence of a kernel vector with positive elements. Hence the rank of $C'$ is 2 and $C'$ has a 1-dimensional kernel, which by virtue of

$$\begin{pmatrix} 1 & \sin\varphi_1 & \sin\varphi_1\sin\varphi_2 + \sigma\cos\varphi_1\cos\varphi_2 \\ \sin\varphi_1 & 1 & \sin\varphi_2 \\ \sin\varphi_1\sin\varphi_2 + \sigma\cos\varphi_1\cos\varphi_2 & \sin\varphi_2 & 1 \end{pmatrix} \begin{pmatrix} \cos\varphi_2 \\ \sin(\sigma\varphi_2 - \varphi_1) \\ -\sigma\cos\varphi_1 \end{pmatrix} = 0 \quad (11)$$

is proportional to $v_\sigma = (\cos\varphi_2, \sin(\sigma\varphi_2 - \varphi_1), -\sigma\cos\varphi_1)^T$. Note that $v_\sigma \neq 0$, since $\varphi_1, \varphi_2$ are not both equal to $\frac{\pi}{2}$. Hence $v_\sigma$ has to have positive elements, which discards the choice $\sigma = 1$ and implies (10). This proves the first part of the lemma.

Let us pass to the second part. By virtue of (11) it is sufficient to show that $C' = D^{-1}CD^{-1}$ is positive semi-definite and of rank 2. This is easily seen by virtue of the factorization

$$\begin{pmatrix} 1 & \sin\varphi_1 & -\cos(\varphi_1 + \varphi_2) \\ \sin\varphi_1 & 1 & \sin\varphi_2 \\ -\cos(\varphi_1 + \varphi_2) & \sin\varphi_2 & 1 \end{pmatrix} = \begin{pmatrix} \cos\varphi_1 & \sin\varphi_1 \\ 0 & 1 \\ -\cos\varphi_2 & \sin\varphi_2 \end{pmatrix} \begin{pmatrix} \cos\varphi_1 & \sin\varphi_1 \\ 0 & 1 \\ -\cos\varphi_2 & \sin\varphi_2 \end{pmatrix}^T. \quad (12)$$

This completes the proof. $\qquad\square$

**Lemma 3.3.** *The following implications hold.*
  *i) (2,3,5) imply (4);*
  *ii) (2,4) imply (3);*
  *iii) (2–4) imply (5).*

*Proof.* i) By (5) we have

$$\begin{aligned} \sin(\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)}) &= -\cos\left(\left|\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} + \frac{\pi}{2}\right|\right) \\ &> \cos(\varphi_{j-2(5)} + \varphi_{j+2(5)}) = -\cos(\pi + \varphi_{j-2(5)} + \varphi_{j+2(5)}). \end{aligned}$$

Both expressions $|\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} + \frac{\pi}{2}|$ and $\pi + \varphi_{j-2(5)} + \varphi_{j+2(5)}$ are contained in the interval $[0, \pi)$ by (2,3), and on this interval the cosine function is monotonely decreasing. It follows that $|\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} + \frac{\pi}{2}| > \pi + \varphi_{j-2(5)} + \varphi_{j+2(5)}$, which for each $j = 1, \ldots, 5$ amounts to the two possibilities

$$\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} - \varphi_{j-2(5)} - \varphi_{j+2(5)} > \frac{\pi}{2}, \qquad \sum_{j=1}^5 \varphi_j < -\frac{3\pi}{2}.$$

Let us prove by contradiction that the second inequality must hold. Assume that $\sum_{j=1}^5 \varphi_j \geq -\frac{3\pi}{2}$, then for all $j = 1, \ldots, 5$ we have $\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} - \varphi_{j-2(5)} - \varphi_{j+2(5)} > \frac{\pi}{2}$. Adding all 5 inequalities together, we arrive at $\sum_{j=1}^5 \varphi_j > \frac{5\pi}{2}$, which contradicts (3). This completes the proof of i).

ii) We have $\varphi_1 + \varphi_2 < -\frac{3\pi}{2} - \varphi_3 - \varphi_4 - \varphi_5 < 0$, where the first inequality holds by (4) and the second one by (2). The other inequalities in (3) are proven similarly.

iii) By (2,3) we have $\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} + \frac{\pi}{2} > -\pi$ and $\pi + \varphi_{j-2(5)} + \varphi_{j+2(5)} \in (0, \pi)$, and by virtue of (4) we have $-(\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} + \frac{\pi}{2}) > \pi + \varphi_{j-2(5)} + \varphi_{j+2(5)} > 0$. Hence both expressions $-(\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} + \frac{\pi}{2})$ and $\pi + \varphi_{j-2(5)} + \varphi_{j+2(5)}$ are in the interval $(0, \pi)$, on which the cosine function is monotonely decreasing. Thus, again by virtue of (4), we have

$$t_j = -\cos\left(\varphi_{j-1(5)} + \varphi_j + \varphi_{j+1(5)} + \frac{\pi}{2}\right) + \cos(\pi + \varphi_{j-2(5)} + \varphi_{j+2(5)}) > 0,$$

yielding (5). $\qquad\square$

**Lemma 3.4.** *Let $\varphi \in \mathbb{R}^5$ satisfy (2–4). Then $\det T(\varphi) > 0$.*

*Proof.* By Lemma 3.3,iii) we have (5). Introduce the complex variables $z_j = e^{i\varphi_j}$, $j = 1, \ldots, 5$. We then get

$$\begin{aligned} t_j &= \frac{z_{j-1(5)} z_j z_{j+1(5)} - z_{j-1(5)}^{-1} z_j^{-1} z_{j+1(5)}^{-1}}{2i} - \frac{z_{j-2(5)} z_{j+2(5)} + z_{j-2(5)}^{-1} z_{j+2(5)}^{-1}}{2} \\ &= \frac{i(iz_{j-1(5)} z_j z_{j+1(5)} + z_{j-2(5)} z_{j+2(5)})(1 + iz_1 z_2 z_3 z_4 z_5)}{2z_1 z_2 z_3 z_4 z_5}. \end{aligned}$$

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This yields

$$\det T(\varphi) = \det \begin{pmatrix} 1 & \frac{z_4-z_4^{-1}}{2i} & -\frac{z_4z_5+z_4^{-1}z_5^{-1}}{2} & -\frac{z_2z_3+z_2^{-1}z_3^{-1}}{2} & \frac{z_3-z_3^{-1}}{2i} \\ \frac{z_4-z_4^{-1}}{2i} & 1 & \frac{z_5-z_5^{-1}}{2i} & -\frac{z_5z_1+z_5^{-1}z_1^{-1}}{2} & -\frac{z_3z_4+z_3^{-1}z_4^{-1}}{2} \\ -\frac{z_4z_5+z_4^{-1}z_5^{-1}}{2} & \frac{z_5-z_5^{-1}}{2i} & 1 & \frac{z_1-z_1^{-1}}{2i} & -\frac{z_1z_2+z_1^{-1}z_2^{-1}}{2} \\ -\frac{z_2z_3+z_2^{-1}z_3^{-1}}{2} & -\frac{z_5z_1+z_5^{-1}z_1^{-1}}{2} & \frac{z_1-z_1^{-1}}{2i} & 1 & \frac{z_2-z_2^{-1}}{2i} \\ \frac{z_3-z_3^{-1}}{2i} & -\frac{z_3z_4+z_3^{-1}z_4^{-1}}{2} & -\frac{z_1z_2+z_1^{-1}z_2^{-1}}{2} & \frac{z_2-z_2^{-1}}{2i} & 1 \end{pmatrix}$$

$$= -\frac{(1+iz_1z_2z_3z_4z_5)^3 \prod_{j=1}^5 (iz_{j-1(5)}z_jz_{j+1(5)} + z_{j-2(5)}z_{j+2(5)})}{16z_1^4z_2^4z_3^4z_4^4z_5^4}$$

$$= t_1t_2t_3t_4t_5 \frac{2iz_1z_2z_3z_4z_5}{(1+iz_1z_2z_3z_4z_5)^2} = \frac{t_1t_2t_3t_4t_5}{1-\sin(\varphi_1+\varphi_2+\varphi_3+\varphi_4+\varphi_5)} > 0,$$

where the last inequality holds by $\sum_j \varphi_j \in (-\frac{5\pi}{2}, -\frac{3\pi}{2})$, as a consequence of (2,4), and by virtue of (5). $\square$

**Lemma 3.5.** *Define a function* $f : \Phi \to \mathbb{R}^5$ *componentwise by* $f_j(\varphi) = \frac{\cos\varphi_j \sin(\varphi_{j-2(5)}+\varphi_{j+2(5)})}{\cos\varphi_{j-1(5)}\cos\varphi_{j+1(5)}}$, $j = 1,\ldots,5$, *where* $\Phi$ *is given by (7). Then the equation* $f(\varphi) = c$, $c \in \mathbb{R}^5$ *a constant vector, has only isolated solutions in* $\Phi$.

*Proof.* By Lemma 3.3,ii) the elements $\varphi \in \Phi$ satisfy all three sets of inequalities (2–4). The Jacobian $\frac{\partial f}{\partial \varphi}$ is given by

$$\begin{pmatrix} -\frac{\sin\varphi_1\sin(\varphi_3+\varphi_4)}{\cos\varphi_5\cos\varphi_2} & \frac{\cos\varphi_1\sin(\varphi_3+\varphi_4)\sin\varphi_2}{\cos\varphi_5\cos^2\varphi_2} & \frac{\cos\varphi_1\cos(\varphi_3+\varphi_4)}{\cos\varphi_5\cos\varphi_2} & \frac{\cos\varphi_1\cos(\varphi_3+\varphi_4)}{\cos\varphi_5\cos\varphi_2} & \frac{\cos\varphi_1\sin(\varphi_3+\varphi_4)\sin\varphi_5}{\cos^2\varphi_5\cos\varphi_2} \\ \frac{\cos\varphi_2\sin(\varphi_4+\varphi_5)\sin\varphi_1}{\cos^2\varphi_1\cos\varphi_3} & -\frac{\sin\varphi_2\sin(\varphi_4+\varphi_5)}{\cos\varphi_1\cos\varphi_3} & \frac{\cos\varphi_2\sin(\varphi_4+\varphi_5)\sin\varphi_3}{\cos\varphi_1\cos^2\varphi_3} & \frac{\cos\varphi_2\cos(\varphi_4+\varphi_5)}{\cos\varphi_1\cos\varphi_3} & \frac{\cos\varphi_2\cos(\varphi_4+\varphi_5)}{\cos\varphi_1\cos\varphi_3} \\ \frac{\cos\varphi_3\cos(\varphi_5+\varphi_1)}{\cos\varphi_2\cos\varphi_4} & \frac{\cos\varphi_3\sin(\varphi_5+\varphi_1)\sin\varphi_2}{\cos^2\varphi_2\cos\varphi_4} & -\frac{\sin\varphi_3\sin(\varphi_5+\varphi_1)}{\cos\varphi_2\cos\varphi_4} & \frac{\cos\varphi_3\sin(\varphi_5+\varphi_1)\sin\varphi_4}{\cos\varphi_2\cos^2\varphi_4} & \frac{\cos\varphi_3\cos(\varphi_5+\varphi_1)}{\cos\varphi_2\cos\varphi_4} \\ \frac{\cos\varphi_4\cos(\varphi_1+\varphi_2)}{\cos\varphi_3\cos\varphi_5} & \frac{\cos\varphi_4\cos(\varphi_1+\varphi_2)}{\cos\varphi_3\cos\varphi_5} & \frac{\cos\varphi_4\sin(\varphi_1+\varphi_2)\sin\varphi_3}{\cos^2\varphi_3\cos\varphi_5} & -\frac{\sin\varphi_4\sin(\varphi_1+\varphi_2)}{\cos\varphi_3\cos\varphi_5} & \frac{\cos\varphi_4\sin(\varphi_1+\varphi_2)\sin\varphi_5}{\cos\varphi_3\cos^2\varphi_5} \\ \frac{\cos\varphi_5\sin(\varphi_2+\varphi_3)\sin\varphi_1}{\cos\varphi_4\cos^2\varphi_1} & \frac{\cos\varphi_5\cos(\varphi_2+\varphi_3)}{\cos\varphi_4\cos\varphi_1} & \frac{\cos\varphi_5\cos(\varphi_2+\varphi_3)}{\cos\varphi_4\cos\varphi_1} & \frac{\cos\varphi_5\sin(\varphi_2+\varphi_3)\sin\varphi_4}{\cos^2\varphi_4\cos\varphi_1} & -\frac{\sin\varphi_5\sin(\varphi_2+\varphi_3)}{\cos\varphi_4\cos\varphi_1} \end{pmatrix}.$$

Introducing complex variables $z_j = e^{i\varphi_j}$ and computing the determinant, we get

$$\det \frac{\partial f}{\partial \varphi} = \frac{16(z_1^2z_2^2z_3^2z_4^2z_5^2+1)^2}{(z_1^2+1)(z_2^2+1)(z_3^2+1)(z_4^2+1)(z_5^2+1)z_1z_2z_3z_4z_5} = \frac{2\cos^2(\varphi_1+\varphi_2+\varphi_3+\varphi_4+\varphi_5)}{\cos\varphi_1\cos\varphi_2\cos\varphi_3\cos\varphi_4\cos\varphi_5} > 0.$$

The last inequality comes from the fact that $\sum_{j=1}^5 \varphi_j \in (-\frac{5\pi}{2}, -\frac{3\pi}{2})$ by virtue of (2,4) and $\varphi_j \in (-\frac{\pi}{2}, \frac{\pi}{2})$ by virtue of (2,3). By the implicit function theorem the function $f$ is hence locally invertible, and its level sets consist of isolated points. $\square$

In the next sections we prove Theorem 3.1.

## 3.1 Proof of the first part

Assume the conditions of the first part of Theorem 3.1. By Theorem 2.3 there exists a permutation matrix $P$ such that $A = PA'P^T$ and $A'$ has exactly 5 isolated zeros $u^1,\ldots,u^5 \in \Delta_5$ with patterns $(11001), (11100), (01110), (00111), (10011)$, respectively. Then by Lemma 2.2 the $3 \times 3$ submatrices $A'_{I_j^3}$ of $A'$ are positive semi-definite for $j = 1,\ldots,5$. Moreover, the set $\{x \in \Delta_3 \mid x^T A'_{I_j^3} x = 0\}$ consists of a single point, namely $u^j_{I_j^3}$. Hence $A'_{I_j^3}$ satisfies the conditions of the first part of Lemma 3.2 and can be represented in the form (8). It follows that $A$ has the structure (6) with $P$ a permutation matrix, $D$ a diagonal matrix with positive diagonal elements, and $\varphi$ satisfying (2,3) by virtue of (9,10). Note also that $T(\varphi)$ is in the orbit of $A$ with respect to $\mathcal{G}_5$ and hence copositive.

It rests to show inequality (4). To this end, we closely follow the argumentation leading to [3, eq. (4.24)]. Consider the upper left $4 \times 4$ submatrix $B = T_{I_5^4}(\varphi)$ of $T(\varphi)$. The matrix $B$ is copositive and by [5, Theorem 2] must be an element of $S_+(4) + NN_4$, i.e., it can be represented as a sum $B' + B''$ with $B' \in S_+(4)$ and $B'' \geq 0$. By (11) the vectors $x = (\cos\varphi_5, -\sin(\varphi_4+\varphi_5), \cos\varphi_4, 0)^T$,

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$x' = (0, \cos\varphi_1, -\sin(\varphi_5 + \varphi_1), \cos\varphi_5)^T$ are zeros of $B$. Since these vectors by (2,3) have nonnegative elements, they must also be zeros of both $B'$ and $B''$ by the copositivity of these summands. It follows that $B''$ can have nonzero elements only in the upper right and lower left corners, and that both $x, x'$ are in the kernel of $B'$. If, however, $B'' = 0$, then $B = B'$, and every convex combination of $x, x'$ is also a zero of $B$ with nonnegative elements. This contradicts the condition that $A$ and hence $T(\varphi)$ has only isolated zeros in $\Delta_5$.

The relation $B'x = 0$ can then be rewritten as follows: there exists $t > 0$ such that

$$
\begin{pmatrix}
1 & \sin\varphi_4 & -\cos(\varphi_4 + \varphi_5) & -\cos(\varphi_2 + \varphi_3) - t \\
\sin\varphi_4 & 1 & \sin\varphi_5 & -\cos(\varphi_5 + \varphi_1) \\
-\cos(\varphi_4 + \varphi_5) & \sin\varphi_5 & 1 & \sin\varphi_1 \\
-\cos(\varphi_2 + \varphi_3) - t & -\cos(\varphi_5 + \varphi_1) & \sin\varphi_1 & 1
\end{pmatrix}
\begin{pmatrix}
\cos\varphi_5 \\
-\sin(\varphi_4 + \varphi_5) \\
\cos\varphi_4 \\
0
\end{pmatrix} = 0,
$$

which yields

$$
\begin{aligned}
t\cos\varphi_5 &= -\cos(\varphi_2 + \varphi_3)\cos\varphi_5 + \cos(\varphi_5 + \varphi_1)\sin(\varphi_4 + \varphi_5) + \sin\varphi_1\cos\varphi_4 \\
&= \cos\varphi_5(-\cos(\varphi_2 + \varphi_3) + \sin(\varphi_1 + \varphi_4 + \varphi_5)).
\end{aligned}
$$

Finally, by virtue of $\cos\varphi_5 > 0$, which is a consequence of (2,3), we get $\sin(\varphi_1 + \varphi_4 + \varphi_5) > \cos(\varphi_2 + \varphi_3)$. Repeating the reasoning for the other submatrices $T_{I_j^4}(\varphi)$, we arrive at all of the inequalities (5). Now (4) follows from Lemma 3.3,i) and the first part of Theorem 3.1 is proven.

## 3.2 Proof of the second part

Assume $A$ is as in the second part of Theorem 3.1. Since the properties of being copositive, extremal, as well as the exclusion conditions in the formulation of Theorem 3.1 are invariant under the action of $\mathcal{G}_5$, we can assume without loss of generality that both $P$ and $D$ are given by the identity matrix, and hence $A = T(\varphi)$. Note that by Lemma 3.3 the quintuple $\varphi$ satisfies all four groups of inequalities (2–5).

### 3.2.1 $A$ is copositive

The first step will be to prove copositivity of the $4 \times 4$ submatrices $A_{I_j^4}$. Let $B = T_{I_5^4}(\varphi)$ as in the previous subsection. We have the representation

$$
\begin{aligned}
B &= \begin{pmatrix}
1 & \sin\varphi_4 & -\cos(\varphi_4 + \varphi_5) & -\sin(\varphi_4 + \varphi_5 + \varphi_1) + t_5 \\
\sin\varphi_4 & 1 & \sin\varphi_5 & -\cos(\varphi_5 + \varphi_1) \\
-\cos(\varphi_4 + \varphi_5) & \sin\varphi_5 & 1 & \sin\varphi_1 \\
-\sin(\varphi_4 + \varphi_5 + \varphi_1) + t_5 & -\cos(\varphi_5 + \varphi_1) & \sin\varphi_1 & 1
\end{pmatrix} \\
&= \begin{pmatrix}
\cos\varphi_4 & \sin\varphi_4 \\
0 & 1 \\
-\cos\varphi_5 & \sin\varphi_5 \\
-\sin(\varphi_1 + \varphi_5) & -\cos(\varphi_1 + \varphi_5)
\end{pmatrix}
\begin{pmatrix}
\cos\varphi_4 & \sin\varphi_4 \\
0 & 1 \\
-\cos\varphi_5 & \sin\varphi_5 \\
-\sin(\varphi_1 + \varphi_5) & -\cos(\varphi_1 + \varphi_5)
\end{pmatrix}^T + t_5 e_{14},
\end{aligned}
$$

where $t_5 = \sin(\varphi_4 + \varphi_5 + \varphi_1) - \cos(\varphi_2 + \varphi_3) > 0$ by Lemma 3.3,iii). Thus $B$ has been represented as a sum of elements in $S_+(4)$ and $NN_4$. This proves copositivity of $B$. By repeating the argument for the other submatrices $A_{I_j^4}$, we likewise prove their copositivity.

We shall now consider the values of the quadratic form $A$ on the compact set $C = \{x \in \mathbb{R}_+^5 \mid ||x||_2 = 1\}$. Since every $4 \times 4$ principal submatrix of $A$ is copositive, the form $A$ is nonnegative on the boundary of $C$. Thus the assumption that $A$ is not copositive implies the existence of a local minimum $x^*$ of the function $f(x) = x^T A x$ in the interior of $C$, with $f(x^*) < 0$. This implies that $x^*$ is an eigenvector of $A$ with negative eigenvalue. However, by Lemma 3.4 the matrix $A$ has at least another negative eigenvalue, and this implies the existence of a path on the shell $||x||_2 = 1$ linking $x^*$ with $-x^*$ on which the form $A$ is strictly negative. But since $-x^* \notin C$, this contradicts the condition that $A$ is nonnegative on the boundary of $C$. Hence $A$ must be copositive.

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### 3.2.2 $A$ is extremal

From (11) it follows that $A$ is zero on the columns $x^1, \ldots, x^5$ of the matrix

$$
\begin{pmatrix}
-\sin(\varphi_3 + \varphi_4) & \cos\varphi_5 & 0 & 0 & \cos\varphi_2 \\
\cos\varphi_3 & -\sin(\varphi_4 + \varphi_5) & \cos\varphi_1 & 0 & 0 \\
0 & \cos\varphi_4 & -\sin(\varphi_5 + \varphi_1) & \cos\varphi_2 & 0 \\
0 & 0 & \cos\varphi_5 & -\sin(\varphi_1 + \varphi_2) & \cos\varphi_3 \\
\cos\varphi_4 & 0 & 0 & \cos\varphi_1 & -\sin(\varphi_2 + \varphi_3)
\end{pmatrix}.
$$

We are done if we show that $A$ is, up to multiplication with a constant, the only copositive form that is zero on these vectors. Let $B$ be another such form. Then the $3 \times 3$ submatrix $B_{I_j^3}$ of $B$ is positive semi-definite by Lemma 2.2. Its kernel contains the vector $x_{I_j^3}^j = (\cos\varphi_{j-2(5)}, -\sin(\varphi_{j-2(5)} + \varphi_{j+2(5)}), \cos\varphi_{j+2(5)})^T$, because $(x_{I_j^3}^j)^T B_{I_j^3} x_{I_j^3}^j = (x^j)^T B x^j = 0$. Note that by virtue of (12) the submatrices $A_{I_j^3}$ have rank 2. By possibly replacing $B$ by a convex combination $\lambda B + (1 - \lambda)A$ with $\lambda > 0$ small enough, we may assume without restriction of generality that the submatrices $\lambda B_{I_j^3} + (1 - \lambda)A_{I_j^3}$ also have rank 2 for all $\lambda \in [0,1]$, and their 1-dimensional kernel is generated by $x_{I_j^3}^j$.

Choose $\lambda \in [0,1]$ and set $C = \lambda B + (1-\lambda)A$. Since all elements of $x_{I_j^3}^j$ are positive, Lemma 3.2 is applicable to the submatrices $C_{I_j^3}$, and $C$ has a representation of the form $D'T(\xi)D'$, where $D' = \operatorname{diag}(d_1', \ldots, d_5')$ with $d_j' > 0$, $j = 1, \ldots, 5$, and $\xi = (\xi_1, \ldots, \xi_5)^T$ satisfies (2,3). Now by the second part of Lemma 3.2 the kernel of $C_{I_j^3}$ is proportional to the vector $(d_{j-1(5)}'^{-1} \cos\xi_{j-2(5)}, -d_j'^{-1} \sin(\xi_{j-2(5)} + \xi_{j+2(5)}), d_{j+1(5)}'^{-1} \cos\xi_{j+2(5)})^T$. Hence there exist constants $\rho_j > 0$, $j = 1, \ldots, 5$, such that for all $j = 1, \ldots, 5$

$$\rho_j d_{j-1(5)}'^{-1} \cos\xi_{j-2(5)} = \cos\varphi_{j-2(5)}, \tag{13}$$

$$-\rho_j d_j'^{-1} \sin(\xi_{j-2(5)} + \xi_{j+2(5)}) = -\sin(\varphi_{j-2(5)} + \varphi_{j+2(5)}), \tag{14}$$

$$\rho_j d_{j+1(5)}'^{-1} \cos\xi_{j+2(5)} = \cos\varphi_{j+2(5)}. \tag{15}$$

Combining (13) for $j$ and (15) for $j' = j + 1(5)$, we obtain the relations $\rho_j d_{j-1(5)}'^{-1} = \rho_{j+1(5)} d_{j+2(5)}'^{-1}$, $j = 1, \ldots, 5$. These 5 relations determine the constants $\rho_j$ up to a common positive factor $\rho$ in dependence of the numbers $d_j'$, namely $\rho_j = \rho d_{j-1(5)}' d_j' d_{j+1(5)}'$. Thus (13,14) become

$$d_{j-2(5)}' \rho d_{j+2(5)}' \cos\xi_j = \cos\varphi_j, \tag{16}$$

$$\rho d_{j-1(5)}' d_{j+1(5)}' \sin(\xi_{j-2(5)} + \xi_{j+2(5)}) = \sin(\varphi_{j-2(5)} + \varphi_{j+2(5)}). \tag{17}$$

Multiplying on the one hand (16) with (17) for $j$, and on the other hand (16) for $j' = j - 1(5)$ and $j'' = j + 1(5)$, and taking the ratio of both products, we obtain for all $j = 1, \ldots, 5$

$$\frac{\cos\xi_j \sin(\xi_{j-2(5)} + \xi_{j+2(5)})}{\cos\xi_{j-1(5)} \cos\xi_{j+1(5)}} = \frac{\cos\varphi_j \sin(\varphi_{j-2(5)} + \varphi_{j+2(5)})}{\cos\varphi_{j-1(5)} \cos\varphi_{j+1(5)}}. \tag{18}$$

Now note that $\xi$ is an explicit continuous function of the elements of $C$, given elementwise by $\xi_j = \arcsin\sqrt{\frac{C_{j-2(5),j+2(5)}^2}{C_{j-2(5),j-2(5)} C_{j+2(5),j+2(5)}}}$. For $\lambda = 0$ we have $C = A$ and hence $\xi = \varphi$, which is indeed a solution of (18). Moreover, by Lemma 3.5 this is the only solution to equation (18) in some neighbourhood of $\varphi$. Therefore $\xi \equiv \varphi$ for all $\lambda \in [0,1]$, because $C$ is continuous in $\lambda$. From (16) we then get $d_{j-2(5)}' d_{j+2(5)}' = \rho^{-1}$ for all $j = 1, \ldots, 5$. Taking the logarithm of these equations, we get a linear system in $\log d_j'$, whose only solution is given by $d_j' = \rho^{-1/2}$ for all $j = 1, \ldots, 5$. Thus $C = \rho^{-1}A$, and $B$ must be proportional to $A$. This proves the extremality of $A$.

### 3.2.3 $A$ satisfies the exclusion properties

From (3) it follows that there exists at least one index $j$ such that $\varphi_j < 0$. This implies $\sin\varphi_j < 0$, so $A = T(\varphi)$ is not nonnegative.

Now recall that by (12) the $3 \times 3$ submatrices $A_{I_j^3}$ have rank 2. If $A$ were positive semi-definite, it could hence not be of full rank, which contradicts Lemma 3.4.

It remains to show that $A$ is not in the orbit of the Horn form. To see this, note that the $2 \times 2$ principal submatrices of $A$ are of full rank by virtue of (2,3), while those of the Horn form are of rank 1, and that this property is invariant under the action of $\mathcal{G}_5$.

This completes the proof of Theorem 3.1.

## 4 Conclusions

Theorems 3.1, 2.1, and the fact that the Horn form is extremal in $\mathcal{C}_5$ [6] furnish an exhaustive description of the generators of the cone $\mathcal{C}_5$. While the orbit of the Horn form and the positive semi-definite extremals form 5-dimensional varieties, the extremals (6) form a 10-dimensional variety, parameterized by the diagonal elements of $D$ and the quintuple of angles $\varphi$. Here for each permutation $P$ we obtain a smooth component of this variety. Since cyclic permutations of the indices and a complete reversal of order yield the same zero pattern in Theorem 2.3 and hence the same smooth component, there exist $5!/10 = 12$ such smooth components.

It is worth noting that the intersection of each smooth component with the affine subspace of matrices all whose diagonal elements equal 1 is homeomorphic to the simplex $\Phi$ given by (7). For $P$ the identity permutation, the vertices of this simplex correspond to the Horn form (for $\varphi_j = -\frac{\pi}{2}$ for all $j = 1, \ldots, 5$) and to positive semi-definite extremals (for the other 5 vertices).

## References

[1] L. D. Baumert. Extreme copositive quadratic forms. *Pacific J. Math.*, 19(2):197–204, 1966.

[2] L. D. Baumert. Extreme copositive quadratic forms. II. *Pacific J. Math.*, 20(1):1–20, 1967.

[3] Leonard Daniel Baumert. *Extreme copositive quadratic forms.* PhD thesis, California Institute of Technology, Pasadena, California, 1965.

[4] Samuel Burer, Kurt Anstreicher, and Mirjam Dür. The difference between $5 \times 5$ doubly nonnegative and completely positive matrices. *Linear Algebra Appl.*, 431:1539–1552, 2009.

[5] P. H. Diananda. On nonnegative forms in real variables some or all of which are nonnegative. *Proc. Cambridge Philos. Soc.*, 58:17–25, 1962.

[6] M. Jr. Hall and M. Newman. Copositive and completely positive quadratic forms. *Proc. Cambridge Philos. Soc.*, 59:329–339, 1963.

[7] A. J. Hoffman and F. Pereira. On copositive matrices with -1,0,1 entries. *J. Comb. Theory A*, 14:302–309, 1973.

[8] Katta G. Murty and Santosh N. Kabadi. Some NP-complete problems in quadratic and nonlinear programming. *Math. Program.*, 39:117–129, 1987.

[9] Changqing Xu. Completely positive matrices of order five. *Acta Math. Appl. Sin.-E.*, 17(4):550–562, 2001.