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Copositive matrices with circulant zero pattern

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Abstract

Let $n \geq 5$ and let $u^1, \dots, u^n$ be nonnegative real n-vectors such that the indices of their positive elements form the sets $\{1, 2, \dots, n-2\}, \{2, 3, \dots, n-1\}, \dots, \{n, 1, \dots, n-3\}$, respectively. Here each index set is obtained from the previous one by a circular shift. The set of copositive forms which vanish on the vectors $u^1, \dots, u^n$ is a face of the copositive cone $\mathcal{C}^n$. We give an explicit semi-definite description of this face and of its subface consisting of positive semi-definite matrices, and study their properties. If the vectors $u^1, \dots, u^n$ and their positive multiples exhaust the zero set of an exceptional copositive form belonging to this face, then we call this form regular, otherwise degenerate. We show that degenerate forms are always extremal, and regular forms can be extremal only if n is odd. We construct explicit examples of extremal degenerate forms for any order $n \geq 5$, and examples of extremal regular forms for any odd order $n \geq 5$. The set of all degenerate forms, i.e., defined by different collections $u^1, \dots, u^n$ of zeros, is a submanifold of codimension $2n$, the set of all regular forms a submanifold of codimension n.

1 Introduction

Let $\mathcal{S}^n$ be the vector space of real symmetric $n \times n$ matrices. In this space, we may define the cone $\mathcal{N}^n$ of element-wise nonnegative matrices, the cone $\mathcal{S}_+^n$ of positive semi-definite matrices, and the cone $\mathcal{C}^n$ of copositive matrices, i.e., matrices $A \in \mathcal{S}^n$ such that $x^T A x \geq 0$ for all $x \in \mathbb{R}_+^n$. Obviously we have $\mathcal{S}_+^n + \mathcal{N}^n \subset \mathcal{C}^n$, but the converse inclusion holds only for $n \leq 4$ [6, Theorem 2]. Copositive matrices which are not elements of the sum $\mathcal{S}_+^n + \mathcal{N}^n$ are called *exceptional*. Copositive matrices play an important role in non-convex and combinatorial optimization, see, e.g., [5] or the surveys [10],[17],[4],[8]. Of particular interest are the exceptional extreme rays of $\mathcal{C}^n$.

A fruitful concept in the study of copositive matrices is that of zeros and their supports, initiated in the works of Baumert [2],[3], see also [16],[7], and [19] for further developments and applications. A non-zero vector $u \in \mathbb{R}_+^n$ is called a *zero* of a copositive matrix $A \in \mathcal{C}^n$ if $u^T A u = 0$. The *support* $\operatorname{supp} u$ of a zero u is the index set of its positive elements.

Note that each of the cones $\mathcal{N}^n$, $\mathcal{S}_+^n$, $\mathcal{C}^n$ is invariant with respect to a simultaneous permutation of the row and column indices, and with respect to a simultaneous pre- and post-multiplication with a positive definite diagonal matrix. These operations generate a group of linear transformations of $\mathcal{S}^n$, which we shall call $\mathcal{G}_n$.

Exceptional copositive matrices first appear at order $n = 5$. The *Horn matrix*

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}, \qquad (1)$$

named after its discoverer Alfred Horn, and the other matrices in its $\mathcal{G}_5$-orbit have been the first examples of exceptional extremal copositive matrices [14]. Any other exceptional extremal matrix in $\mathcal{C}^5$ lies in the

$\mathcal{G}_5$-orbit of a matrix

$$T(\theta) = \begin{pmatrix} 1 & -\cos\theta_1 & \cos(\theta_1+\theta_2) & \cos(\theta_4+\theta_5) & -\cos\theta_5 \\ -\cos\theta_1 & 1 & -\cos\theta_2 & \cos(\theta_2+\theta_3) & \cos(\theta_5+\theta_1) \\ \cos(\theta_1+\theta_2) & -\cos\theta_2 & 1 & -\cos\theta_3 & \cos(\theta_3+\theta_4) \\ \cos(\theta_4+\theta_5) & \cos(\theta_2+\theta_3) & -\cos\theta_3 & 1 & -\cos\theta_4 \\ -\cos\theta_5 & \cos(\theta_5+\theta_1) & \cos(\theta_3+\theta_4) & -\cos\theta_4 & 1 \end{pmatrix} \quad (2)$$

for some angles $\theta_k \in (0,\pi)$ satisfying $\sum_{k=1}^5 \theta_k < \pi$ [15, Theorem 3.1]. Both the Horn matrix H and the matrices $T(\theta)$ possess zeros with supports $\{1,2,3\},\{2,3,4\},\{3,4,5\},\{4,5,1\},\{5,1,2\}$, respectively. Note that these supports are exactly the vertex subsets obtained by removing the vertices of a single edge in the cycle graph C_5.

In this contribution we shall generalize the exceptional extremal elements of $\mathcal{C}^5$ to arbitrary order $n \geq 5$ by taking the above property of the supports as our point of departure. Fix a set $\mathbf{u} = \{u^1,\dots,u^n\} \subset \mathbb{R}_+^n$ of nonnegative vectors with supports $\{1,2,\dots,n-2\},\{2,3,\dots,n-1\},\dots,\{n,1,\dots,n-3\}$, respectively, i.e., the supports of the vectors u^j are the vertex subsets obtained by removing the vertices of a single edge in the cycle graph C_n. We then consider the faces

$$F_{\mathbf{u}} = \{A \in \mathcal{C}^n \mid (u^j)^T A u^j = 0 \;\forall\, j = 1,\dots,n\},$$
$$P_{\mathbf{u}} = \{A \in \mathcal{S}_+^n \mid (u^j)^T A u^j = 0 \;\forall\, j = 1,\dots,n\}$$

of the copositive cone and the positive semi-definite cone, respectively. Note that $P_{\mathbf{u}} \subset F_{\mathbf{u}}$.

One of our main results is an explicit semi-definite description of the faces $F_{\mathbf{u}}$ and $P_{\mathbf{u}}$ (Theorem 2). In order to obtain this description, we associate the set $\mathbf{u}$ to a discrete-time linear dynamical system $\mathbf{S_u}$ of order $d = n-3$ and with time-dependent coefficients having period n. If $\mathcal{L}_{\mathbf{u}}$ is the d-dimensional solution space of this system, then there exists a canonical bijective linear map between $F_{\mathbf{u}}$ and the set of positive semi-definite symmetric bilinear forms on the dual space $\mathcal{L}_{\mathbf{u}}^*$ satisfying certain additional homogeneous linear equalities and inequalities. For an arbitrary collection $\mathbf{u}$ in general only the zero form satisfies the corresponding linear matrix inequality (LMI) and the face $F_{\mathbf{u}}$ consists of the zero matrix only. However, for every $n \geq 5$ there exist collections $\mathbf{u}$ for which the LMI has non-trivial feasible sets.

The properties of the copositive matrices in $F_{\mathbf{u}}$ are closely linked to the properties of the periodic linear dynamical system $\mathbf{S_u}$. Such systems are the subject of *Floquet theory*, see, e.g., [11, Section 3.4]. We need only the concept of the *monodromy matrix* and its eigenvalues, the *Floquet multipliers*, which we shall review in Section 3. We show that the face $P_{\mathbf{u}}$ is isomorphic to $\mathcal{S}_+^{d_1}$, where d_1 is the geometric multiplicity of the Floquet multiplier 1, or equivalently, the dimension of the subspace of n-periodic solutions of $\mathbf{S_u}$. For the existence of exceptional copositive matrices in $F_{\mathbf{u}}$ it is necessary that all or all but one Floquet multiplier are located on the unit circle (Corollary 7).

We are able to describe the structure of $F_{\mathbf{u}}$ explicitly in general. Exceptional matrices $A \in F_{\mathbf{u}}$ can be divided in two categories. If every zero of A is proportional to one of the zeros $u^1,\dots,u^n$, then we call the copositive matrix A *regular*, otherwise we call it *degenerate*[1]. We show that degenerate matrices are always extremal, while regular matrices can be extremal only for odd n. For even n a regular matrix can be represented as a non-trivial sum of a degenerate matrix and a positive semi-definite rank 1 matrix, the corresponding face $F_{\mathbf{u}}$ is then isomorphic to $\mathbb{R}_+^2$. For odd n a sufficient condition for extremality of a regular matrix is that -1 does not appear among the Floquet multipliers (Theorem 3). For every

[1] The terms *regular* and *degenerate* are used in this very specific sense in this paper. The motivation is that whether an exceptional matrix $A \in F_{\mathbf{u}}$ is regular or degenerate depends on whether certain principal submatrices of A of size $n-3$ are regular or degenerate in the ordinary sense.

$n \geq 5$ the degenerate matrices constitute an algebraic submanifold of $\mathcal{S}^n$ of codimension $2n$ (Theorem 6), while the regular matrices form an algebraic submanifold of codimension n (Theorem 4), in which the extremal matrices form an open subset (Theorem 5).

Finally, in Section 7.2 we construct explicit examples of circulant (i.e., invariant with respect to simultaneous circular shifts of row and column indices) exceptional extremal copositive matrices, both degenerate and regular. We also give an exhaustive description of all degenerate exceptional matrices for order $n = 6$ in Section 8. Some auxiliary results whose proofs would interrupt the flow of exposition are collected in two appendices.

1.1 Further notations

For $n \geq 5$ an integer, define the ordered index sets $I_1 = (1, 2, \dots, n-2)$, $I_2 = (2, 3, \dots, n-1), \dots, I_n = (n, 1, \dots, n-3)$ of cardinality $n-2$, each obtained by a circular shift of the indices from the previous one. We will need also the index sets $I'_1 = (1, 2, \dots, n-3), \dots, I'_n = (n, 1, \dots, n-4)$ defined similarly.

Let $k > 0$ be an integer. For a vector $u \in \mathbb{R}^k$, a $k \times k$ matrix M, and an ordered index set $I \subset \{1, \dots, k\}$ of cardinality $|I|$, we shall denote by u_i the i-th entry of u, by u_I the subvector $(u_i)_{i \in I} \in \mathbb{R}^{|I|}$ of u composed of the elements with index in the ordered set I, by M_{ij} the (i,j)-th entry of M, and by M_I the principal submatrix $(M_{ij})_{i,j \in I} \in \mathbb{R}^{|I| \times |I|}$ of M composed of the elements having row and column index in I.

In order to distinguish it from the index sets $I_1, \dots, I_n$ defined above, we shall denote the identity matrix or the identity operator by Id or Id_k if it is necessary to indicate the size of the matrix. Denote by $E_{ij} \in \mathcal{N}^n$ the matrix which has ones at the positions (i,j) and (j,i) and zeros elsewhere. For a real number r, we denote by $\lfloor r \rfloor$ the largest integer not exceeding r and by $\lceil r \rceil$ the smallest integer not smaller than r.

Definition 1. Let $A \in \mathcal{C}^n$ be an exceptional copositive matrix possessing zeros $u^1, \dots, u^n \in \mathbb{R}^n_+$ such that $\operatorname{supp} u^j = I_j$, $j = 1, \dots, n$. We call the matrix A *regular* if every zero v of A is proportional to one of the zeros $u^1, \dots, u^n$, and we call it *degenerate* otherwise.

2 Conditions for copositivity

In this section we consider matrices $A \in \mathcal{S}^n$ such that the submatrices $A_{I_1}, \dots, A_{I_n}$ are all positive semi-definite and possess element-wise positive kernel vectors. We derive necessary and sufficient conditions for such a matrix to be copositive. The goal of the section is to prove Theorem 1 below. We start with a few simple auxiliary lemmas.

Lemma 1. *[9, Lemma 2.4] Let $A \in \mathcal{C}_n$ and let u be a zero of A. Then the principal submatrix $A_{\operatorname{supp} u}$ is positive semi-definite.*

Lemma 2. *[2, p.200] Let $A \in \mathcal{C}_n$ and let u be a zero of A. Then $Au \geq 0$ element-wise.*

Lemma 3. *Let $n \geq 5$, and let $i, j \in \{1, \dots, n\}$ be arbitrary indices. Then there exists $k \in \{1, \dots, n\}$ such that $i, j \in I_k$.*

Proof. For every index $i \in \{1, \dots, n\}$, there exist exactly two indices k such that $i \notin I_k$. The assertion of the lemma then follows from the Dirichlet principle. □

Corollary 1. *Let $n \geq 5$ and let $A \in \mathcal{C}^n$ have zeros $u^1, \dots, u^n$ with supports $I_1, \dots, I_n$, respectively. Then for every pair of indices $i, j \in \{1, \dots, n\}$, the matrix $A - \varepsilon E_{ij}$ is not copositive for every $\varepsilon > 0$.*

Proof. Let $i, j \in \{1, \dots, n\}$. By Lemma 3 there exists a zero u^k of A such that $i, j \in \operatorname{supp} u^k$. The assertion then follows by $(u^k)^T(A - \varepsilon E_{ij})u^k < 0$ for every $\varepsilon > 0$, see [3, p. 10]. □

Corollary 2. *[2, Corollary 3.7] Let $A \in \mathcal{C}^n$ be such that $A - \varepsilon E_{ij}$ is not copositive for every $\varepsilon > 0$ and all $i, j = 1, \dots, n$. If A has a zero with support of cardinality $n - 1$, then A is positive semi-definite.*

A zero $u \in \mathbb{R}^n_+$ of A is called *minimal* if there is no other zero $v \in \mathbb{R}^n_+$ of A such that the inclusion $\operatorname{supp} v \subset \operatorname{supp} u$ is strict. For a fixed copositive matrix, the number of its minimal zeros whose elements sum up to 1 is finite [16, Corollary 3.6]. The next result furnishes a criterion involving minimal zeros to check whether a copositive matrix is extremal.

Lemma 4. *[7, Theorem 17] Let $A \in \mathcal{C}^n$, and let $u^1, \dots, u^m$ be its minimal zeros whose elements sum up to 1. Then A is extremal if and only if the solution space of the linear system of equations on the matrix $X \in \mathcal{S}^n$ given by*

$$(Xu^j)_i = 0 \qquad \forall\, i, j: \ (Au^j)_i = 0$$

is one-dimensional (and hence generated by A).

Lemma 5. *[16, Lemma 4.3] Let $A \in \mathcal{C}_n$ be a copositive matrix and let $w \in \mathbb{R}^n$. Then there exists $\varepsilon > 0$ such that $A - \varepsilon ww^T$ is copositive if and only if $\langle w, u \rangle = 0$ for all zeros u of A.*

These results allow us to prove the following theorem on matrices $A \in \mathcal{S}^n$ having zeros $u^1, \dots, u^n$ with supports $I_1, \dots, I_n$, respectively.

Theorem 1. *Let $n \geq 5$ and let $A \in \mathcal{S}^n$ be such that for every $j = 1, \dots, n$ there exists a nonnegative vector u^j with $\operatorname{supp} u^j = I_j$ satisfying $(u^j)^T A u^j = 0$. Then the following are equivalent:*

(i) A is copositive;
(ii) every principal submatrix of A of size $n - 1$ is copositive;
(iii) every principal submatrix of A of size $n - 1$ is in $\mathcal{S}^{n-1}_+ + \mathcal{N}^{n-1}$;
(iv) A_{I_j} is positive semi-definite for $j = 1, \dots, n$, $(u^n)^T A u^1 \geq 0$, and $(u^j)^T A u^{j+1} \geq 0$ for $j = 1, \dots, n - 1$.

Moreover, given above conditions (i)—(iv), the following are equivalent:

(a) A is positive semi-definite;
(b) at least one of the n numbers $(u^n)^T A u^1$ and $(u^j)^T A u^{j+1}$, $j = 1, \dots, n - 1$, is zero;
(c) all n numbers $(u^n)^T A u^1$ and $(u^j)^T A u^{j+1}$, $j = 1, \dots, n - 1$, are zero;
(d) A is not exceptional.

Proof. (i) ⇒ (iv) is a consequence of Lemmas 1 and 2.

(iv) ⇒ (iii) is a consequence of Lemma 29 in the Appendix, applied to the $(n - 1) \times (n - 1)$ principal submatrices of A.

(iii) ⇒ (ii) is trivial.

(ii) $\Rightarrow$ (i): Let $\Delta = \{v = (v_1, \dots, v_n)^T \in \mathbb{R}^n_+ \mid \sum_{j=1}^n v_j = 1\}$ be the standard simplex. By (ii) the quadratic form A is nonnegative on $\partial\Delta$. On $\partial\Delta$ it then reaches its global minimum 0 at appropriate positive multiples $\alpha_j u^j \in \Delta$ of the zeros u^j for all $j = 1, \dots, n$. Since the line segment connecting $\alpha_1 u^1$ and $\alpha_2 u^2$ still lies in $\partial\Delta$, the quadratic function $Q(v) = v^T A v$ cannot be strictly convex on Δ. But then it reaches its global minimum over Δ on the boundary $\partial\Delta$. This minimum over Δ then also equals 0, which proves the copositivity of A.

We have shown the equivalence of conditions (i)—(iv). Let us now assume that A satisfies (i)—(iv) and pass to the second part of the theorem.

(a) $\Rightarrow$ (c): If $A \succeq 0$, then all vectors u^j, $j = 1, \dots, n$, are in the kernel of A. This implies (c).

(c) $\Rightarrow$ (b) is trivial.

(b) $\Rightarrow$ (a): Without loss of generality, let $(u^1)^T A u^2 = 0$. It then follows that $u_+ = u^1 + u^2$ is also a zero of A, with $\operatorname{supp} u_+ = \{1, \dots, n-1\}$. By Corollaries 1 and 2 A is then positive semi-definite, which proves (a).

(a) $\Rightarrow$ (d) holds by definition.

(d) $\Rightarrow$ (a): Assume that A can be written as a sum $A = P + N$ with $P \in \mathcal{S}^n_+$ and $N \in \mathcal{N}^n$. By Corollary 1 none of the elements of N can be positive and hence $A = P$, implying (a). $\square$

Let us comment on Theorem 1. It states that the presence of n zeros with supports I_j, $j = 1, \dots, n$ place stringent constraints on a copositive matrix $A \in \mathcal{C}^n$. Such a matrix must either be exceptional or positive semi-definite. Which of these two cases arises is determined by any of the n numbers in condition (iv) of the theorem, which are either simultaneously positive or simultaneously zero.

3 Linear systems with periodic coefficients

In this section we investigate the solution spaces of linear periodic dynamical systems and perform some linear algebraic constructions on them. These will be later put in correspondence to copositive forms. First we shall introduce the monodromy and the Floquet multipliers associated with such systems, for further reading about these and related concepts see, e.g., [11, Section 3.4].

We consider real scalar discrete-time homogeneous linear dynamical systems governed by the equation

$$x_{t+d} + \sum_{i=0}^{d-1} c_i^t x_{t+i} = \sum_{i=0}^{d} c_i^t x_{t+i} = 0, \qquad t = 1, 2, \dots. \tag{3}$$

Here $x_t \in \mathbb{R}$ is the value of the solution x at time instant t, $d > 0$ is the order, and $c^t = (c_0^t, \dots, c_d^t)^T \in \mathbb{R}^{d+1}$, $t \geq 1$, are the coefficient vectors of the system. For convenience we have set $c_d^t = 1$ for all $t \geq 1$. We assume that the coefficients are periodic with period $n > d$, i.e., $c^{t+n} = c^t$ for all $t \geq 1$. Denote by $\mathcal{L}$ the linear space of all solutions $x = (x_t)_{t\geq 1}$. This space has dimension d and can be parameterized, e.g., by the vector $(x_1, \dots, x_d) \in \mathbb{R}^d$ of initial conditions.

If $x = (x_t)_{t\geq 1}$ is a solution of the system, then $y = (x_{t+n})_{t\geq 1}$ is also a solution by the periodicity of the coefficients. The corresponding linear map $\mathfrak{M} : \mathcal{L} \to \mathcal{L}$ taking x to y is called the *monodromy* of the periodic system. Its eigenvalues are called *Floquet multipliers*. The following result is a trivial consequence of this definition.

Lemma 6. *Let $\mathcal{L}_{per} \subset \mathcal{L}$ be the subspace of n-periodic solutions of system* (3)*. Then $x \in \mathcal{L}_{per}$ if and only if x is an eigenvector of the monodromy operator $\mathfrak{M}$ with eigenvalue 1. In particular, $\dim \mathcal{L}_{per}$ equals the geometric multiplicity of the eigenvalue 1 of $\mathfrak{M}$.* □

System (3) is time-reversible if and only if $c_0^t \neq 0$ for all $t = 1, \dots, n$, in this case we may express x_t as a function of $x_{t+1}, \dots, x_{t+d}$. In fact, the following result holds.

Lemma 7. *The determinant of the monodromy matrix is given by $\det \mathfrak{M} = (-1)^{nd} \prod_{t=1}^n c_0^t$.*

Proof. From (3) it follows that the determinant of the linear map taking the vector $(x_t, x_{t+1}, \dots, x_{t+d-1})$ to $(x_{t+1}, \dots, x_{t+d})$ equals $(-1)^d c_0^t$. Iterating this map for $t = 1, \dots, n$, we get that the determinant of the linear map taking the vector $(x_1, \dots, x_d)$ to $(x_{n+1}, \dots, x_{n+d})$ equals $(-1)^{nd} \prod_{t=1}^n c_0^t$. The claim now follows from the fact that the vector $(x_1, \dots, x_d)$ parameterizes the solution space $\mathcal{L}$. □

Let us now consider the space $\mathcal{L}^*$ of linear functionals on the solution space $\mathcal{L}$. For every $t \geq 1$, the map taking a solution $x = (x_s)_{s \geq 1}$ to its value x_t at time instant t is such a linear functional. We shall denote this evaluation functional by $\mathbf{e}_t \in \mathcal{L}^*$. By definition of the monodromy we have $\mathbf{e}_{t+n} = \mathfrak{M}^* \mathbf{e}_t$ for all $t \geq 1$, where $\mathfrak{M}^* : \mathcal{L}^* \to \mathcal{L}^*$ is the adjoint of $\mathfrak{M}$. Moreover,

$$\sum_{i=0}^d c_i^t \mathbf{e}_{t+i} = 0 \qquad \forall\, t \geq 1 \tag{4}$$

as a consequence of (3).

Our main tool in the study of copositive forms in this paper are positive semi-definite symmetric bilinear forms B on $\mathcal{L}^*$ which are invariant with respect to a time shift by the period n, i.e.,

$$B(\mathbf{e}_{t+n}, \mathbf{e}_{s+n}) = B(\mathbf{e}_t, \mathbf{e}_s) \qquad \forall\, t, s \geq 1. \tag{5}$$

Definition 2. We call a symmetric bilinear form B on $\mathcal{L}^*$ satisfying relation (5) a *shift-invariant* form.

Lemma 8. *Assume above notations. A symmetric bilinear form B on $\mathcal{L}^*$ is shift-invariant if and only if it is preserved by the adjoint of the monodromy, i.e., $B(w, w') = B(\mathfrak{M}^* w, \mathfrak{M}^* w')$ for all $w, w' \in \mathcal{L}^*$. An equivalent set of conditions is given by $B(\mathbf{e}_{t+n}, \mathbf{e}_{s+n}) = B(\mathbf{e}_t, \mathbf{e}_s)$ for all $t, s \in \{1, \dots, d\}$.*

Proof. The assertions hold because the evaluation functionals $\mathbf{e}_1, \dots, \mathbf{e}_d$ form a basis of $\mathcal{L}^*$ and $\mathbf{e}_{t+n} = \mathfrak{M}^* \mathbf{e}_t$ for all $t \geq 1$. □

The shift-invariant forms are hence determined by a finite number of linear homogeneous equations and constitute a linear subspace of the space of symmetric bilinear forms on $\mathcal{L}^*$.

The space of symmetric bilinear forms on $\mathcal{L}^*$ can be viewed as the space of symmetric contra-variant second order tensors over $\mathcal{L}$, i.e., it is the linear hull of tensor products of the form $x \otimes x$, $x \in \mathcal{L}$. It is well-known that a symmetric bilinear form can be diagonalized, i.e., represented as a finite sum $B = \sum_{k=1}^r \sigma_k x^k \otimes x^k$ with $\sigma_k \in \{-1, +1\}$, $x^k \in \mathcal{L}$, $k = 1, \dots, r$, the vectors x^k being linearly independent. The vectors x^k in this decomposition are not unique, but their number r and their linear hull depend only on B and are called the *rank* $\operatorname{rk} B$ and the *image* $Im\, B$ of B, respectively. The form is positive semi-definite if all coefficients σ_k in its decomposition equal 1.

Lemma 9. *Let B be a shift-invariant symmetric positive semi-definite bilinear form B on $\mathcal{L}^*$, of rank r. Then there exist at least r (possibly complex) linearly independent eigenvectors of $\mathfrak{M}$ with eigenvalues on the unit circle.*

Proof. Let $B = \sum_{k=1}^r x^k \otimes x^k$ be a decomposition of B as above and complete the linearly independent set $\{x^1, \dots, x^r\}$ to a basis $\{x^1, \dots, x^n\}$ of $\mathcal{L}$. In the coordinates defined by this basis and its dual basis in $\mathcal{L}^*$ the form B is then given by the diagonal matrix $\mathrm{diag}(Id_r, 0, \dots, 0)$. Let M be the coefficient matrix of $\mathfrak{M}$ in this basis, partitioned into submatrices $M_{11}, M_{12}, M_{21}, M_{22}$ corresponding to the partition of the basis into subsets $\{x^1, \dots, x^r\}$ and $\{x^{r+1}, \dots, x^n\}$. Then by Lemma 8 the shift-invariance of B is equivalent to the condition

$$\begin{pmatrix} Id_r & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} Id_r & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}^T = \begin{pmatrix} M_{11}M_{11}^T & M_{11}M_{21}^T \\ M_{21}M_{11}^T & M_{21}M_{21}^T \end{pmatrix}.$$

It follows that $M_{21} = 0$ and M_{11} is an $r \times r$ orthogonal matrix. However, it is well-known that orthogonal matrices possess a full basis of eigenvectors with eigenvalues on the unit circle. The assertion of the lemma now readily follows. □

4 Copositive matrices and linear periodic systems

In this section we establish a relation between the objects considered in the preceding two sections. Throughout this and the next section, we fix a collection $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}_+^n$ of nonnegative vectors such that $\mathrm{supp}\, u^j = I_j$, $j = 1, \dots, n$. Moreover, we assume these vectors are normalized such that the last elements of their positive subvectors $u^j_{I_j}$ all equal 1. To the collection $\mathbf{u}$ we associate a discrete-time linear periodic system $\mathbf{S_u}$ of order $d = n - 3$ and with period n, given by (3) with coefficient vectors $c^t = u^t_{I_t}$, $t = 1, \dots, n$. The coefficient vectors c^t for all other time instants $t > n$ are then determined by the periodicity relation $c^{t+n} = c^t$. Equivalently, the dynamics of $\mathbf{S_u}$ is given by the equations

$$\sum_{i=0}^d u_s^{t'} x_{t+i} = 0, \qquad t \geq 1, \tag{6}$$

where $t', s \in \{1, \dots, n\}$ are the unique indices such that $t \equiv t'$ and $t + i \equiv s$ modulo n. Relation (4) then becomes

$$\sum_{i=0}^d u_s^{t'} \mathbf{e}_{t+i} = 0, \qquad \forall\, t \geq 1, \tag{7}$$

with t', s defined as above.

By Lemma 7 the monodromy of $\mathbf{S_u}$ then satisfies

$$\det \mathfrak{M} = \prod_{j=1}^n u_j^j > 0. \tag{8}$$

In particular, the system $\mathbf{S_u}$ is time-reversible. Denote by $\mathcal{L}_\mathbf{u}$ the space of solutions of $\mathbf{S_u}$.

Let $\mathcal{A}_\mathbf{u} \subset \mathcal{S}^n$ be the linear subspace of matrices A satisfying $A_{I_j} u^j_{I_j} = A_{I_j} c^j = 0$ for all $j = 1, \dots, n$. To $A \in \mathcal{A}_\mathbf{u}$ we associate a symmetric bilinear form B on the dual space $\mathcal{L}_\mathbf{u}^*$ by setting $B(\mathbf{e}_t, \mathbf{e}_s) = A_{ts}$ for every $t, s = 1, \dots, d$ and defining the value of B on arbitrary vectors in $\mathcal{L}_\mathbf{u}^*$ by linear extension. In other words, in the basis $\{\mathbf{e}_1, \dots, \mathbf{e}_d\}$ of $\mathcal{L}_\mathbf{u}^*$ the coefficient matrix of B is given by the submatrix $A_{I'_1}$. Let $\Lambda : A \mapsto B$ be the so-defined linear map from $\mathcal{A}_\mathbf{u}$ into the space of symmetric bilinear forms on $\mathcal{L}_\mathbf{u}^*$. Our first step will be to describe the image of Λ. To this end, we need the following lemma.

Lemma 10. *Let $A \in \mathcal{A}_{\mathbf{u}}$ and $B = \Lambda(A)$. Then for every integer $r \geq 1$, the $(n-2) \times (n-2)$-matrix $B_r = (B(\mathbf{e}_{t+r}, \mathbf{e}_{s+r}))_{t,s=0,\dots,d}$ equals the submatrix $A_{I_{r'}}$, where $r' \in \{1, \dots, n\}$ is the unique index satisfying $r \equiv r'$ modulo n. Equivalently,*

$$B(\mathbf{e}_t, \mathbf{e}_s) = A_{t's'} \qquad \forall\, t, s \geq 1 : \ |t - s| \leq n - 3, \tag{9}$$

where $t', s' \in \{1, \dots, n\}$ are the unique indices such that $t \equiv t'$, $s' \equiv s$ modulo n.

Proof. We proceed by induction over r. By definition of Λ the upper left $(n-3) \times (n-3)$ submatrix of B_1 equals the corresponding submatrix of A_{I_1}. However, we have $A_{I_1} c^1 = 0$ by virtue of $A \in \mathcal{A}_{\mathbf{u}}$ and $B_1 c^1 = 0$ by virtue of (4) for $t = 1$. Hence the difference $A_{I_1} - B_1$ is a symmetric matrix, with possibly non-zero elements only in the last row or in the last column, which possesses a kernel vector with all elements positive. It is easily seen that this difference must then be the zero matrix, proving the assertion of the lemma for $r = 1$.

The induction step from $r - 1$ to r proceeds in a similar manner, with equality of the upper left $(n-3) \times (n-3)$ submatrices of B_r and $A_{I_{r'}}$ now guaranteed by the induction hypothesis. □

The lemma asserts that the submatrices $A_{I_1}, \dots, A_{I_n}$ are all of the form $(B(\mathbf{e}_t, \mathbf{e}_s))_{t,s \in I}$ for certain index sets I. Some of their properties are hence determined by the corresponding properties of B.

Corollary 3. *Let $A \in \mathcal{A}_{\mathbf{u}}$ and $B = \Lambda(A)$. Then the ranks of the matrices A_{I_j}, $j = 1, \dots, n$, and of all their submatrices of size $(n-3) \times (n-3)$, are equal to the rank of the symmetric bilinear form B.*

Proof. Since the system $\mathbf{S}_{\mathbf{u}}$ is time-reversible, the evaluation operators $\mathbf{e}_t, \dots, \mathbf{e}_{t+d-1}$ form a basis of $\mathcal{L}_{\mathbf{u}}^*$ for every $t \geq 1$. On the other hand, the operators $\mathbf{e}_t, \dots, \mathbf{e}_{t+d}$ are linearly dependent for all $t \geq 1$, the dependence being given by (7). All coefficients in this relation are non-zero, hence any of the operators $\mathbf{e}_t, \dots, \mathbf{e}_{t+d}$ can be expressed as a linear combination of the d other operators. It follows that every subset of $\{\mathbf{e}_t, \dots, \mathbf{e}_{t+d}\}$ of cardinality d is a basis of $\mathcal{L}_{\mathbf{u}}^*$. Therefore the $d \times d$ matrix $(B(\mathbf{e}_s, \mathbf{e}_{s'}))_{s \in I, s' \in I'}$, where I, I' are such subsets, has rank equal to $\operatorname{rk} B$. The same holds for the matrices $(B(\mathbf{e}_s, \mathbf{e}_{s'}))_{s,s'=t,\dots,t+d}$ for all $t \geq 1$. The corollary now follows from Lemma 10. □

Corollary 4. *Let $A \in \mathcal{A}_{\mathbf{u}}$ and $B = \Lambda(A)$. Then the symmetric bilinear form B is shift-invariant and satisfies the linear relations*

$$B(\mathbf{e}_t, \mathbf{e}_s) = B(\mathbf{e}_{t+n}, \mathbf{e}_s) \qquad \forall\, t, s \geq 1 : \ 3 \leq s - t \leq n - 3. \tag{10}$$

Proof. By (9) we have $B(\mathbf{e}_t, \mathbf{e}_s) = A_{ts} = B(\mathbf{e}_{t+n}, \mathbf{e}_{s+n})$ for all $t, s = 1, \dots, d$. This in turn implies the shift-invariance of B by Lemma 8.

The inequalities $3 \leq s - t \leq n - 3$ imply $|t - s| \leq n - 3$, $|t + n - s| \leq n - 3$. Relations (10) then follow from (9) in a similar way as the shift-invariance. □

Now we are ready to describe the image of the map Λ.

Lemma 11. *Suppose that $n \geq 5$. Then the linear map Λ is injective, and its image consists of those shift-invariant symmetric bilinear forms B on $\mathcal{L}_{\mathbf{u}}^*$ which satisfy relations* (10).

Proof. In view of Corollary 4 it suffices to show that for every shift-invariant symmetric bilinear form B satisfying (10) there exists a unique matrix $A \in \mathcal{A}_{\mathbf{u}}$ such that $B = \Lambda(A)$.

Let B be such a form. We define the corresponding matrix A as follows. Let $i, j \in \{1, \dots, n\}$ be arbitrary indices such that $i \leq j$. Put

$$A_{ij} = A_{ji} = \begin{cases} B(\mathbf{e}_i, \mathbf{e}_j), & j - i \leq n - 3; \\ B(\mathbf{e}_{i+n}, \mathbf{e}_j), & j - i > n - 3. \end{cases} \qquad (11)$$

The shift-invariance of B and relations (10) then imply (9). This gives $B_r = (B(\mathbf{e}_{t+r}, \mathbf{e}_{s+r}))_{t,s=0,\dots,d} = A_{I_r}$ for every $r = 1, \dots, n$. Now $B_r c^r = 0$ by virtue of (4), which implies $A_{I_r} c^r = 0$ and hence $A \in \mathcal{A}_{\mathbf{u}}$. Moreover, $\Lambda(A) = B$ by construction of A.

Uniqueness of A follows from Lemmas 10 and 3. □

Now we shall investigate which symmetric bilinear forms B in the image of Λ are the images of copositive matrices. First we consider positive semi-definite bilinear symmetric forms B.

Lemma 12. *Suppose $n \geq 5$ and let $A \in \mathcal{A}_{\mathbf{u}}$ and $B = \Lambda(A)$. Then the following are equivalent:*

(i) the form B is positive semi-definite;
(ii) the submatrices A_{I_j} are positive semi-definite for all $j = 1, \dots, n$;
(iii) any of the submatrices A_{I_j}, $j = 1, \dots, n$, is positive semi-definite.

Moreover, given above conditions (i)—(iii), the following holds:

(a) the difference $B(\mathbf{e}_n, \mathbf{e}_{n-2}) - B(\mathbf{e}_n, \mathbf{e}_{2n-2})$ has the same sign as $(u^n)^T A u^1$;
(b) the difference $B(\mathbf{e}_{j+n}, \mathbf{e}_{j+n-2}) - B(\mathbf{e}_{j+n}, \mathbf{e}_{j+2n-2})$ has the same sign as $(u^j)^T A u^{j+1}$, $j = 1, 2$;
(c) the difference $B(\mathbf{e}_j, \mathbf{e}_{j-2}) - B(\mathbf{e}_j, \mathbf{e}_{j+n-2})$ has the same sign as $(u^j)^T A u^{j+1}$, $j = 3, \dots, n-1$.

Proof. The first part of the lemma is a direct consequence of Lemma 10 and of the fact that the set $\{\mathbf{e}_t, \dots, \mathbf{e}_{t+d}\}$ spans the whole space $\mathcal{L}_{\mathbf{u}}^*$ for all $t \geq 1$.

Let us prove the second part and assume conditions (i)—(iii). Consider the $(n-1) \times (n-1)$ matrix $A_{(1,\dots,n-1)}$. By Lemma 10 its upper left and its lower right principal submatrix of size $n-2$ coincides with the matrix $(B(\mathbf{e}_t, \mathbf{e}_s))_{t,s \in I}$ with $I = \{1, \dots, n-2\}$ and $I = \{2, \dots, n-1\}$, respectively. Hence it can be written as a sum $(B(\mathbf{e}_t, \mathbf{e}_s))_{t,s=1,\dots,n-1} + \delta E_{1,n-1}$ for some real δ. Note that the first summand is positive semi-definite by condition (i). On the other hand, $A_{1,n-1} = B(\mathbf{e}_{n+1}, \mathbf{e}_{n-1})$ by (9). Hence $\delta = B(\mathbf{e}_{n+1}, \mathbf{e}_{n-1}) - B(\mathbf{e}_1, \mathbf{e}_{n-1}) = B(\mathbf{e}_{n+1}, \mathbf{e}_{n-1}) - B(\mathbf{e}_{n+1}, \mathbf{e}_{2n-1})$, where the second equality follows from the shift-invariance of B which is in turn a consequence of Lemma 11. By virtue of Lemma 29 we then get (b) for $j = 1$.

The other assertions of the second part are proven in a similar way by starting with the remaining $(n-1) \times (n-1)$ principal submatrices of A. □

Lemma 13. *Let $n \geq 5$, and let $A \in \mathcal{C}^n$ be such that $(u^j)^T A u^j = 0$ for all $j = 1, \dots, n$. Then $A \in \mathcal{A}_{\mathbf{u}}$, and $B = \Lambda(A)$ is positive semi-definite and satisfies the inequalities*

$$B(\mathbf{e}_t, \mathbf{e}_{t+2}) \geq B(\mathbf{e}_{t+n}, \mathbf{e}_{t+2}) \qquad \forall t \geq 1. \qquad (12)$$

Moreover, either B satisfies all inequalities (12) *with equality, namely when A is positive semi-definite, or all inequalities* (12) *are strict, namely when A is exceptional.*

Proof. Let $A \in \mathcal{C}^n$ such that $(u^j)^T A u^j = 0$ for all $j = 1,\dots,n$. Then $A_{I_j} \succeq 0$ for $j = 1,\dots,n$ by Lemma 1. The relation $(c^j)^T A_{I_j} c^j = (u^j)^T A u^j = 0$ then implies $A_{I_j} c^j = 0$ for all $j = 1,\dots,n$, and we get indeed $A \in \mathcal{A}_{\mathbf{u}}$. By Lemma 12 we then have $B \succeq 0$. From Theorem 1 and Lemma 12 we obtain (12) for $t = 1,\dots,n$, with equality or strict inequality for positive semi-definite or exceptional A, respectively. For all other $t > n$ these relations follow by the shift-invariance of B which in turn is implied by Corollary 4. □

Lemma 14. *Let B be a positive semi-definite symmetric bilinear form in the image of Λ which satisfies inequalities* (12)*. Then its pre-image $A = \Lambda^{-1}(B)$ is copositive and satisfies $(u^j)^T A u^j = 0$ for all $j = 1,\dots,n$.*

Proof. Let B be as required, and let A be its pre-image, which is well-defined by Lemma 11. By Lemma 12 the submatrices A_{I_j} are positive semi-definite for all $j = 1,\dots,n$. From $A \in \mathcal{A}_{\mathbf{u}}$ it follows that $(u^j)^T A u^j = 0$ for all $j = 1,\dots,n$. Finally, by Lemma 12 (12) implies the inequalities $(u^n)^T A u^1 \geq 0$ and $(u^j)^T A u^{j+1} \geq 0$, $j = 1,\dots,n-1$. Therefore $A \in \mathcal{C}^n$ by Theorem 1. □

Now we are in a position to describe the faces $F_{\mathbf{u}} = \{A \in \mathcal{C}^n \mid (u^j)^T A u^j = 0 \ \forall\, j = 1,\dots,n\}$ of the copositive cone and $P_{\mathbf{u}} = \{A \in \mathcal{S}_+^n \mid (u^j)^T A u^j = 0 \ \forall\, j = 1,\dots,n\}$ of the positive semi-definite cone which are defined by the zeros u^j, by linear matrix inequalities.

Theorem 2. *Let $n \geq 5$, and let $\mathcal{F}_{\mathbf{u}}$ be the set of positive semi-definite symmetric bilinear forms B on $\mathcal{L}_{\mathbf{u}}^*$ satisfying the linear equality relations*

$$\begin{aligned} B(\mathbf{e}_t, \mathbf{e}_s) &= B(\mathfrak{M}^*\mathbf{e}_t, \mathfrak{M}^*\mathbf{e}_s), && t, s = 1,\dots,n-3; \\ B(\mathbf{e}_t, \mathbf{e}_s) &= B(\mathfrak{M}^*\mathbf{e}_t, \mathbf{e}_s), && 1 \leq t < s \leq n:\ 3 \leq s - t \leq n-3 \end{aligned}$$

and the linear inequalities

$$B(\mathbf{e}_t, \mathbf{e}_{t+2}) \geq B(\mathfrak{M}^*\mathbf{e}_t, \mathbf{e}_{t+2}), \qquad t = 1,\dots,n.$$

Let $\mathcal{P}_{\mathbf{u}} \subset \mathcal{F}_{\mathbf{u}}$ be the subset of forms B which satisfy all linear inequalities with equality.

Then the face of $\mathcal{C}^n$ defined by the zeros u^j, $j = 1,\dots,n$, is given by $F_{\mathbf{u}} = \Lambda^{-1}[\mathcal{F}_{\mathbf{u}}]$, and the face of $\mathcal{S}_+^n$ defined by these zeros is given by $P_{\mathbf{u}} = \Lambda^{-1}[\mathcal{P}_{\mathbf{u}}]$. Moreover, for all forms $B \in \mathcal{F}_{\mathbf{u}} \setminus \mathcal{P}_{\mathbf{u}}$ the linear inequalities are satisfied strictly, and $F_{\mathbf{u}} \setminus P_{\mathbf{u}}$ consists of exceptional matrices.

Proof. By virtue of Lemmas 11, 13, and 14 we have only to show that the finite number of equalities and inequalities stated in the formulation of the theorem are necessary and sufficient to ensure the infinite number of equalities and inequalities in (5),(10),(12). Necessity is evident, since the relations in the theorem are a subset of relations (5),(10),(12).

Sufficiency of the first set of equalities in the theorem to ensure (5) follows from Lemma 8. By the resulting shift-invariance of B it is also sufficient to constrain the index t to $1,\dots,n$ in (10). Now suppose that $t \in \{1,\dots,n\}$, $s > n$, and $3 \leq s-t \leq n-3$. We then have $B(\mathbf{e}_t, \mathbf{e}_s) = B(\mathbf{e}_s, \mathbf{e}_t)$, $B(\mathbf{e}_{t+n}, \mathbf{e}_s) = B(\mathbf{e}_t, \mathbf{e}_{s-n}) = B(\mathbf{e}_{s-n}, \mathbf{e}_t)$. Relation (10) for the index pair (t,s) is hence equivalent to the same relation for the index pair $(t', s') = (s-n, t)$, which also satisfies $1 \leq t' \leq n$ and $3 \leq s' - t' \leq n-3$. For the latter index pair we now have $s' \leq n$, however. Thus (10) also follows from the linear equalities in the theorem. Finally, the set of inequalities in the theorem implies (12) by the shift-invariance of B. □

Corollary 5. *Let $r_{\max}$ be the rank achieved by the forms in the (relative) interior of $\mathcal{F}_{\mathbf{u}}$. Then for every $B \in \partial\mathcal{F}_{\mathbf{u}} \setminus \mathcal{P}_{\mathbf{u}}$ we have* $\mathrm{rk}\ B < r_{\max}$.

Proof. Let $B \in \partial\mathcal{F}_{\mathbf{u}} \setminus \mathcal{P}_{\mathbf{u}}$, and let B' be a form in the relative interior of $\mathcal{F}_{\mathbf{u}}$. Let l be the line segment connecting B with B'. When we reach the boundary point B by moving along l, either a rank drop must occur or one of the linear inequalities must become active. However, the second case cannot happen, because $B \notin \mathcal{P}_{\mathbf{u}}$. □

If the vectors in the collection $\mathbf{u}$ are in generic position, then the set $\mathcal{F}_{\mathbf{u}}$ defined in Theorem 2 consists of the zero form only. In the next section we investigate the consequences of a non-trivial set $\mathcal{F}_{\mathbf{u}}$.

5 Structure of the cones $\mathcal{F}_{\mathbf{u}}$ and $\mathcal{P}_{\mathbf{u}}$

As was mentioned in the introduction, the eigenvalues of the monodromy $\mathfrak{M}$, the Floquet multipliers, largely determine the properties of the matrices in the face $F_{\mathbf{u}}$ of $\mathcal{C}^n$. In this section we shall investigate these connections in detail. In particular, we will be interested in the structure of the cones $P_{\mathbf{u}}$ and $\mathcal{P}_{\mathbf{u}} = \Lambda[P_{\mathbf{u}}]$ defined by the positive semi-definite matrices in the face $F_{\mathbf{u}} \subset \mathcal{C}^n$ and its connections to the periodic solutions of the system $\mathbf{S_u}$. We also investigate the properties of the regular and the degenerate exceptional copositive matrices as defined in Definition 1.

Denote by $\mathcal{L}_{per} \subset \mathcal{L}_{\mathbf{u}}$ the subspace of n-periodic solutions. We have the following characterization of $\mathcal{L}_{per}$.

Lemma 15. *An n-periodic infinite sequence $x = (x_1, x_2, \dots)$ is a solution of $\mathbf{S_u}$ if and only if the vector $(x_1, \dots, x_n)^T \in \mathbb{R}^n$ is orthogonal to all vectors u^j, $j = 1, \dots, n$. In particular, the dimension of $\mathcal{L}_{per}$ equals the corank of the $n \times n$ matrix U composed of the column vectors $u^1, \dots, u^n$.*

Proof. From the n-periodicity of x it follows that (6) are exactly the orthogonality relations between $(x_1, \dots, x_n)^T$ and u^j. The lemma now readily follows. □

We are now in a position to describe the set $\mathcal{P}_{\mathbf{u}}$ in terms of the subspace $\mathcal{L}_{per}$.

Lemma 16. *Suppose that $n \geq 5$. Then $\mathcal{P}_{\mathbf{u}}$ equals the convex hull of all tensor products $x \otimes x$, $x \in \mathcal{L}_{per}$. In particular, $\mathcal{P}_{\mathbf{u}} \simeq \mathcal{S}_+^{\dim \mathcal{L}_{per}}$, and for every $B \in \mathcal{P}_{\mathbf{u}}$ we have $Im\, B \subset \mathcal{L}_{per}$. Moreover, for every $B \in \mathcal{P}_{\mathbf{u}}$ the preimage $A = \Lambda^{-1}(B)$ is given by $A = (B(\mathbf{e}_t, \mathbf{e}_s))_{t,s=1,\dots,n}$.*

Proof. Assume $x \in \mathcal{L}_{per}$ and set $B = x \otimes x$. The n-periodicity of the solution x implies that $x_{t+n} = x_t$ for all $t \geq 1$. For every $t, s \geq 1$ we then have $B(\mathbf{e}_t, \mathbf{e}_s) = x_t x_s = x_{t+n} x_s = B(\mathbf{e}_{t+n}, \mathbf{e}_s)$, which yields (10) and (12) with equality. In a similar way we obtain (5), and hence $B \in \mathcal{P}_{\mathbf{u}}$. Moreover, (11) yields $A = \Lambda^{-1}(B) = (B(\mathbf{e}_t, \mathbf{e}_s))_{t,s=1,\dots,n}$.

By convexity of $\mathcal{P}_{\mathbf{u}}$ it follows that the convex hull of the set $\{x \otimes x \,|\, x \in \mathcal{L}_{per}\}$ is a subset of $\mathcal{P}_{\mathbf{u}}$, and by linearity the above expression for $A = \Lambda^{-1}(B)$ holds also for every B in this convex hull.

Let us prove the converse inclusion. Let $B \in \mathcal{P}_{\mathbf{u}}$ be arbitrary and set $A = \Lambda^{-1}(B)$. Then $A \in P_{\mathbf{u}}$ by Theorem 2. Since $A \succeq 0$ and $(u^j)^T A u^j = 0$, it follows that $Au^j = 0$ for all $j = 1, \dots, n$. Therefore A is in the convex hull of the set $\{vv^T \,|\, \langle v, u^j \rangle = 0 \;\forall\, j = 1, \dots, n\}$. It hence suffices to show that for every $v \in \mathbb{R}^n$ such that $\langle v, u^j \rangle = 0$, $j = 1, \dots, n$, we have $\Lambda(vv^T) = x \otimes x$ for some $x \in \mathcal{L}_{per}$.

Let $v \in \mathbb{R}^n$ be orthogonal to all zeros u^j. By Lemma 15 the n-periodic sequence $x = (x_1, x_2, \dots)$ defined by the initial conditions $x_i = v_i$, $i = 1, \dots, n$, is an n-periodic solution of $\mathbf{S_u}$, $x \in \mathcal{L}_{per}$. But $\Lambda(vv^T) = x \otimes x$ by construction. This completes the proof. □

We now consider the ranks of the forms in $\mathcal{F}_\mathbf{u}$ and $\mathcal{P}_\mathbf{u}$. Let $r_{\max}$ be the maximal rank achieved by forms in $\mathcal{F}_\mathbf{u}$, and r_{PSD} the maximal rank achieved by forms in $\mathcal{P}_\mathbf{u}$.

Corollary 6. *Suppose $n \geq 5$. Then r_{PSD} equals the geometric multiplicity of the eigenvalue 1 of the monodromy operator $\mathfrak{M}$ of the dynamical system $\mathbf{S_u}$.*

Proof. The corollary follows from Lemmas 6 and 16. □

Lemma 17. *Let $n \geq 5$, and let $B \in \mathcal{F}_\mathbf{u} \setminus \mathcal{P}_\mathbf{u}$. Then for every $k \geq 1$ the matrix*

$$\begin{aligned} M_k &= (B(\mathbf{e}_{t+k} - \mathbf{e}_{t+n+k}, \mathbf{e}_{s+k}))_{t=0,\dots,n-5;s=2,\dots,n-3} \\ &= (B((Id - \mathfrak{M}^*)\mathbf{e}_{t+k}, \mathbf{e}_{s+k}))_{t=0,\dots,n-5;s=2,\dots,n-3} \end{aligned}$$

has full rank $n-4$.

Proof. By Lemma 13 the form B satisfies inequalities (12) strictly, which implies that M_k has all diagonal elements positive. By (10) M_k is lower-triangular, and hence has full rank $n-4$. □

Corollary 7. *Let $n \geq 5$, and let $B \in \mathcal{F}_\mathbf{u} \setminus \mathcal{P}_\mathbf{u}$. Then the bilinear form on $\mathcal{L}_\mathbf{u}^*$ given by $(w, w') \mapsto B((Id - \mathfrak{M}^*)w, w')$ has corank at most 1. In particular, both B and $Id - \mathfrak{M}^*$ have corank at most 1. Moreover, $\mathfrak{M}$ has at least $n-4$ linearly independent eigenvectors with eigenvalues on the unit circle.*

Proof. The bilinear form in the statement of the lemma has at least the same rank, namely $n-4$, as the matrices M_k in Lemma 17. Hence it has corank at most 1. It follows that B has corank at most 1, and the proof is concluded by application of Lemma 9. □

Corollary 8. *Suppose $n \geq 5$. If $\mathcal{F}_\mathbf{u} \neq \mathcal{P}_\mathbf{u}$, then $r_{\max} - r_{PSD} \geq n-4$. In particular, in this case $r_{PSD} \leq 1$ and either $r_{\max} = n-4$ or $r_{\max} = n-3$.*

Proof. Let $B \in \mathcal{F}_\mathbf{u} \setminus \mathcal{P}_\mathbf{u}$. Suppose there exists $B' \in \mathcal{P}_\mathbf{u}$ such that $B \succeq B'$. Then also $B - B' \in \mathcal{F}_\mathbf{u} \setminus \mathcal{P}_\mathbf{u}$. Therefore we may assume without loss of generality that there does not exist a non-zero $B' \in \mathcal{P}_\mathbf{u}$ such that $B - B' \succeq 0$. By Lemma 16 we then have $Im\, B \cap \mathcal{L}_{per} = \{0\}$, and hence for every $B' \in \mathcal{P}_\mathbf{u}$ we get $\mathrm{rk}(B + B') = \mathrm{rk}\ B + \mathrm{rk}\ B'$, again by Lemma 16.

Let now $B' \in \mathcal{P}_\mathbf{u}$ such that $\mathrm{rk}\ B' = r_{PSD}$. By Corollary 7 we have $\mathrm{rk}\ B \geq n-4$, and hence $r_{\max} \geq \mathrm{rk}\ B + \mathrm{rk}\ B' = n - 4 + r_{PSD}$. This completes the proof. □

These results allow us to completely characterize the face $F_\mathbf{u}$ in the case when $\mathcal{F}_\mathbf{u}$ does not contain positive definite forms.

Lemma 18. *Suppose $n \geq 5$ and assume $r_{\max} = n-4$. Then either $F_\mathbf{u}$ consists of positive semi-definite matrices only, or $F_\mathbf{u}$ is 1-dimensional and generated by an extremal exceptional copositive matrix A. In the latter case the submatrices A_{I_j} of this exceptional matrix have corank 2 for all $j = 1, \dots, n$.*

Proof. By Corollaries 5 and 7 we have the inclusion $\partial\mathcal{F}_\mathbf{u} \subset \mathcal{P}_\mathbf{u}$. Therefore either $\mathcal{F}_\mathbf{u} = \mathcal{P}_\mathbf{u}$, or $\mathcal{F}_\mathbf{u}$ is 1-dimensional and $\mathcal{P}_\mathbf{u} = \{0\}$. The first claim of the lemma now follows from Theorem 2. The second claim then follows from Corollary 3. □

We shall now concentrate on the case when $\mathcal{F}_{\mathbf{u}}$ contains positive definite forms, i.e., the maximal rank achieved by matrices in $\mathcal{F}_{\mathbf{u}}$ equals $r_{\max} = d = n - 3$.

Lemma 19. *Let $n \geq 5$. Then the following are equivalent:*

(i) the set $\mathcal{F}_{\mathbf{u}}$ contains a positive definite form and $\mathcal{F}_{\mathbf{u}} = \mathcal{P}_{\mathbf{u}}$;
(ii) the monodromy operator $\mathfrak{M}$ of the system $\mathbf{S}_{\mathbf{u}}$ equals the identity;
(iii) the rank of the $n \times n$ matrix U with columns $u^1, \dots, u^n$ equals 3.

Proof. Assume (ii). The LMIs in Theorem 2 reduce to the condition $B \succeq 0$, and hence $\mathcal{F}_{\mathbf{u}} = \mathcal{P}_{\mathbf{u}} = \mathcal{S}_+^{n-3}$, implying (i).

Assume (i). We have $r_{\max} = r_{PSD} = n - 3$, and (ii) follows from Corollary 6.

By Lemma 6 we have $\mathfrak{M} = Id$ if and only if $\dim \mathcal{L}_{per} = n - 3$. By Lemma 15 this is equivalent to the condition $\operatorname{rk} U = 3$, which proves (ii) ⇔ (iii). □

In order to treat the case $r_{\max} = n - 3$ and $\mathcal{F}_{\mathbf{u}} \neq \mathcal{P}_{\mathbf{u}}$ we shall distinguish between odd and even orders n.

Lemma 20. *Let $n > 5$ be even, and suppose $r_{\max} = n - 3$ and $\mathcal{F}_{\mathbf{u}} \neq \mathcal{P}_{\mathbf{u}}$. Then $F_{\mathbf{u}}$ is linearly isomorphic to $\mathbb{R}_+^2$, where one boundary ray of $F_{\mathbf{u}}$ is generated by a rank 1 positive semi-definite matrix, and the other boundary ray is generated by an extremal exceptional copositive matrix A. The submatrices A_{I_j} of this exceptional matrix have corank 2 for all $j = 1, \dots, n$.*

Proof. By Lemma 9 all eigenvalues of the monodromy $\mathfrak{M}$ of the system $\mathbf{S}_{\mathbf{u}}$ lie on the unit circle and their geometric and algebraic multiplicities coincide. However, since $\mathfrak{M}$ is real, its complex eigenvalues are grouped into complex-conjugate pairs. Since the dimension $d = n-3$ of $\mathcal{L}_{\mathbf{u}}^*$ is odd, there must be exactly one real eigenvalue with an odd multiplicity. By (8) this eigenvalue equals 1. Hence r_{PSD} is odd by Corollary 6, but cannot exceed 1 by Corollary 8. Therefore $\dim \mathcal{L}_{per} = 1$ and $\dim \mathcal{P}_{\mathbf{u}} = \dim P_{\mathbf{u}} = 1$, and $P_{\mathbf{u}}$ is generated by a rank 1 positive semi-definite matrix A_P.

Denote the 1-dimensional eigenspace of $\mathfrak{M}^*$ to the eigenvalue 1 by W_1, and let $\mathcal{L}_{per}^{\perp} \subset \mathcal{L}_{\mathbf{u}}^*$ be the orthogonal complement of $\mathcal{L}_{per}$. Then $\mathcal{L}_{per}^{\perp}$ is an invariant subspace of $\mathfrak{M}^*$ and $\mathcal{L}_{\mathbf{u}}^* = W_1 + \mathcal{L}_{per}^{\perp}$. Let now $w^1 \in W_1$ and $w \in \mathcal{L}_{per}^{\perp}$ be arbitrary vectors. Then for every $B \in \mathcal{F}_{\mathbf{u}}$ we get by the shift-invariance $B(w^1, w) = B(\mathfrak{M}^* w^1, \mathfrak{M}^* w) = B(w^1, \mathfrak{M}^* w)$, and hence $B(w^1, (Id - \mathfrak{M}^*)w) = 0$ for all $w \in \mathcal{L}_{per}^{\perp}$. But $(Id - \mathfrak{M}^*)[\mathcal{L}_{per}^{\perp}] = \mathcal{L}_{per}^{\perp}$, because $\mathcal{L}_{per}^{\perp}$ is an invariant subspace of $Id - \mathfrak{M}^*$ and it has a zero intersection with the kernel W_1 of $Id - \mathfrak{M}^*$. It follows that W_1 and $\mathcal{L}_{per}^{\perp}$ are orthogonal under B.

This implies that every $B \in \mathcal{F}_{\mathbf{u}}$ can in a unique way be decomposed into a sum $B = B' + P$ of positive semi-definite forms, with $P \in \mathcal{P}_{\mathbf{u}}$ and $W_1 \subset \ker B'$. Moreover, for every $B \in \mathcal{F}_{\mathbf{u}}$ the corresponding summand B' is also in $\mathcal{F}_{\mathbf{u}}$, because P satisfies inequalities (12) with equality. Thus the cone $\mathcal{F}_{\mathbf{u}}$ splits into a direct sum $\mathcal{F}'_{\mathbf{u}} + \mathcal{P}_{\mathbf{u}}$, where $\mathcal{F}'_{\mathbf{u}} = \{B \in \mathcal{F}_{\mathbf{u}} \mid W_1 \subset \ker B\}$.

By assumption $\mathcal{F}'_{\mathbf{u}} \neq \{0\}$. Any non-zero form in $\mathcal{F}'_{\mathbf{u}}$ lies in $\partial \mathcal{F}_{\mathbf{u}} \setminus \mathcal{P}_{\mathbf{u}}$ and hence must be rank deficient by Corollary 5. On the other hand, any such form has corank at most 1 by Corollary 7, and hence its rank equals $n - 4$. Thus the rank is constant over all forms in $\mathcal{F}'_{\mathbf{u}} \setminus \{0\}$ and inequalities (12) are satisfied strictly. Hence $\mathcal{F}'_{\mathbf{u}} \setminus \{0\}$ must be contained in the relative interior of $\mathcal{F}'_{\mathbf{u}}$, which implies that $\mathcal{F}'_{\mathbf{u}}$ is a ray generated by a single form B'. By Theorem 2 $A' = \Lambda^{-1}(B')$ is then an exceptional extremal copositive matrix, and $F_{\mathbf{u}} \simeq \mathbb{R}_+^2$ is generated by A' and A_P. Since $\operatorname{rk} B' = n - 4$, the submatrices A'_{I_j} also have rank $n - 4$ by Corollary 3, and hence corank 2. □

Lemma 21. *Let $n \geq 5$ be odd, and suppose $r_{\max} = n - 3$ and $\mathcal{F}_{\mathbf{u}} \neq \mathcal{P}_{\mathbf{u}}$. Then $F_{\mathbf{u}}$ does not contain non-zero positive semi-definite matrices.*

If $F_{\mathbf{u}}$ is 1-dimensional, then it is generated by an extremal exceptional copositive matrix A such that the submatrices A_{I_j} have corank 1 for all $j = 1, \dots, n$.

If $\dim F_{\mathbf{u}} > 1$, then the monodromy $\mathfrak{M}$ of the system $\mathbf{S}_{\mathbf{u}}$ possesses the eigenvalue -1, and all boundary rays of $F_{\mathbf{u}}$ are generated by extremal exceptional copositive matrices. For any such boundary matrix A, its submatrices A_{I_j} have corank 2 for all $j = 1, \dots, n$.

Proof. As in the proof of the previous lemma, $\mathfrak{M}$ has all eigenvalues on the unit circle, with equal geometric and algebraic multiplicities. However, now $\dim \mathcal{L}_{\mathbf{u}}^* = n - 3$ is even, and by (8) the real eigenvalues ± 1, if they appear, have even multiplicity. By Corollaries 6 and 8 the multiplicity of the eigenvalue 1 cannot exceed 1 and this eigenvalue does not appear. By Lemma 16 we get $\mathcal{P}_{\mathbf{u}} = \{0\}$ and by Theorem 2 the face $F_{\mathbf{u}}$ does not contain non-zero positive semi-definite matrices.

Suppose now that $F_{\mathbf{u}}$ is not 1-dimensional. Then $\partial\mathcal{F}_{\mathbf{u}} \setminus \mathcal{P}_{\mathbf{u}} = \partial\mathcal{F}_{\mathbf{u}} \setminus \{0\}$ is not empty and by Corollary 5 consists of rank deficient forms. On the other hand, the rank can drop at most by 1 by virtue of Corollary 7. Hence $\dim \ker B = 1$ for all $B \in \partial\mathcal{F}_{\mathbf{u}} \setminus \{0\}$. This kernel must be a real eigenspace of $\mathfrak{M}^*$, because $\mathfrak{M}^*$ preserves the form B by shift-invariance. Therefore $\mathfrak{M}^*$ must have a real eigenvalue, which can only be equal to -1. Moreover, since the boundary subset $\partial\mathcal{F}_{\mathbf{u}} \setminus \{0\}$ consists of forms of corank 1, it must be smooth and every boundary ray is extremal. Indeed, if $\partial\mathcal{F}_{\mathbf{u}}$ would contain a face of dimension exceeding 1, then the boundary of this face would be different from $\{0\}$, but no further rank drop could occur there. Hence the pre-image $\Lambda^{-1}[\partial\mathcal{F}_{\mathbf{u}} \setminus \{0\}]$ consists of extremal exceptional copositive matrices. By Corollary 3 the submatrices A_{I_j} of such a matrix A have rank $n - 4$, or corank 2, for all $j = 1, \dots, n$.

If, on the contrary, $\dim F_{\mathbf{u}} = 1$, then $F_{\mathbf{u}}$ is generated by an extremal exceptional copositive matrix A. By assumption the form $B = \Lambda(A)$ is positive definite and has rank $n - 3$. By Corollary 3 the submatrices A_{I_j} also have rank $n - 3$ for all $j = 1, \dots, n$. □

Finally, we shall investigate the zero set of exceptional copositive matrices $A \in F_{\mathbf{u}}$.

Lemma 22. *Suppose $n \geq 5$, and let $A \in F_{\mathbf{u}}$ be an exceptional copositive matrix. If $v \in \mathbb{R}_+^n$ is a zero of A, then there exists an index $j \in \{1, \dots, n\}$ such that $\operatorname{supp} v \subset I_j$.*

Proof. Since A is exceptional, we cannot have $\operatorname{supp} v = \{1, \dots, n\}$ by Lemma 1. Therefore $\operatorname{supp} v$ is a subset of $\{1, \dots, n\} \setminus \{k\}$ for some $k \in \{1, \dots, n\}$. Without loss of generality, assume that $\operatorname{supp} v \subset \{1, \dots, n-1\}$. By Theorem 1 we have $(u^1)^T A u^2 > 0$, and hence by Lemma 29 we have $A_{(1,\dots,n-1)} = P + \delta E_{1,n-1}$ for some positive semi-definite matrix $P \in \mathcal{S}_+^{n-1}$ and some $\delta > 0$. Since v is a zero of A, we get that the subvector $v_{(1,\dots,n-1)} \in \mathbb{R}_+^{n-1}$ is a zero of both P and $E_{1,n-1}$. It follows that the first and the last element of this subvector cannot be simultaneously positive, which implies $\operatorname{supp} v \subset I_1$ or $\operatorname{supp} v \subset I_2$. □

Theorem 3. *Let $A \in F_{\mathbf{u}}$ be an exceptional copositive matrix and set $B = \Lambda(A)$. Then either*

- *(i.a)* *A is regular;*
- *(i.b)* *B is positive definite;*
- *(i.c)* *the corank of the submatrices A_{I_j} equals 1, $j = 1, \dots, n$;*
- *(i.d)* *the minimal zero pattern of A is $\{I_1, \dots, I_n\}$, with minimal zeros $u^1, \dots, u^n$;*

(i.e) *for even n the matrix A is the sum of a degenerate exceptional copositive matrix and a rank 1 positive semi-definite matrix;*

(i.f) *if n is odd and the monodromy operator $\mathfrak{M}$ has no eigenvalue equal to -1, then A is extremal;*

or

(ii.a) *A is degenerate;*

(ii.b) *the corank of B equals 1;*

(ii.c) *the corank of the submatrices A_{I_j} equals 2, $j = 1, \dots, n$;*

(ii.d) *the support of any minimal zero of A is a strict subset of one of the index sets $I_1, \dots, I_n$, and every index set I_j has exactly two subsets which are supports of minimal zeros of A;*

(ii.e) *every non-minimal zero of A has support equal to I_j for some $j = 1, \dots, n$ and is a sum of two minimal zeros;*

(ii.f) *A is extremal.*

Proof. By Corollary 7 the form B is either positive definite or has corank 1. By Corollary 3 the submatrices A_{I_j} have corank 1 in the first case and corank 2 in the second case, for all $j = 1, \dots, n$. Hence the zeros u^j are minimal in the first case and not minimal in the second case, for all $j = 1, \dots, n$. By Lemma 22 A is regular in the first case, and there are no index sets other than $I_1, \dots, I_n$ which are supports of minimal zeros of A. Thus either (i.a)—(i.d) or (ii.a)—(ii.c) hold.

Assume the second case. By Lemma 22 every support of a minimal zero of A is then a strict subset of one of the sets $I_1, \dots, I_n$. The set of zeros v of A satisfying $\operatorname{supp} v \subset I_j$ is determined by the intersection of the two-dimensional kernel of A_{I_j} with the nonnegative orthant. However, every two-dimensional convex cone is linearly isomorphic to $\mathbb{R}_+^2$ and is hence the convex hull of two extreme rays. Assertions (ii.d),(ii.e) then readily follow. The maximal rank achieved by forms in $\mathcal{F}_{\mathbf{u}}$ equals either $n - 4$ or $n - 3$ by Corollary 8. In the first case (ii.f) follows from Lemma 18, in the second case from Lemma 20 or 21, dependent on the parity of n.

Assume (i.a)—(i.d). Then (i.e) and (i.f) follow from Lemmas 20 and 21, respectively. □

The prototype of exceptional copositive matrices satisfying conditions (i.a)—(i.f) are the T-matrices (2), while the prototype of those satisfying (ii.a)—(ii.f) is the Horn matrix (1).

6 Submanifolds of extremal exceptional copositive matrices

In the previous two sections we considered the face $F_{\mathbf{u}} \subset \mathcal{C}^n$ for a fixed collection $\mathbf{u}$ of zeros. In Theorem 3 we have shown that there are two potential possibilities for an exceptional copositive matrix A in such a face $F_{\mathbf{u}}$. Namely, either A is regular, or A is degenerate, either imposing its own set of conditions on A. In this section we show that in each of these cases, the matrix A is embedded in a submanifold of codimension n or $2n$, respectively, which consists of exceptional copositive matrices with similar properties. However, different matrices in this submanifold may belong to faces $F_{\mathbf{u}}$ corresponding to different collections $\mathbf{u}$. Recall that regular and degenerate are understood in the sense of Definition 1.

Theorem 4. *Let $n \geq 5$, and let $\hat{A} \in \mathcal{C}^n$ be a regular exceptional matrix with zeros $\hat{u}^1, \dots, \hat{u}^n \in \mathbb{R}_+^n$ such that $\operatorname{supp} \hat{u}^j = I_j$. Then there exists a neighbourhood $\mathcal{U} \subset \mathcal{S}^n$ of $\hat{A}$ with the following properties:*

(i) *if $A \in \mathcal{U}$ and $\det A_{I_j} = 0$ for all $j = 1, \dots, n$, then A is a regular exceptional copositive matrix;*

(ii) *the set of matrices $A \in \mathcal{U}$ satisfying the conditions in (i) is an algebraic submanifold of codimension n in $\mathcal{S}^n$.*

Proof. By Theorem 3 the submatrices $\hat{A}_{I_j}$ have rank $n-3$ for $j = 1, \dots, n$. Let A be sufficiently close to $\hat{A}$ and such that $\det A_{I_j} = 0$ for all $j = 1, \dots, n$. The submatrix A_{I_j} has $n-3$ positive eigenvalues by continuity and one zero eigenvalue by assumption, and hence is positive semi-definite for all $j = 1, \dots, n$. Moreover, the kernel of A_{I_j} is close to the kernel of $\hat{A}_{I_j}$ and hence is generated by an element-wise positive vector for all $j = 1, \dots, n$. We then find vectors $u^1, \dots, u^n \in \mathbb{R}^n_+$, close to $\hat{u}^1, \dots, \hat{u}^n$, such that $\operatorname{supp} u^j = I_j$ and the subvector $u^j_{I_j}$ is in the kernel of A_{I_j}. Then $(u^j)^T A u^j = 0$ for all $j = 1, \dots, n$, and $(u^j)^T A u^k$ is close to $(\hat{u}^j)^T \hat{A} \hat{u}^k$ for all $j, k = 1, \dots, n$. By Theorem 1 we have $(\hat{u}^n)^T \hat{A} \hat{u}^1 > 0$, $(\hat{u}^j)^T \hat{A} \hat{u}^{j+1} > 0$, $j = 1, \dots, n-1$, and hence also $(u^n)^T A u^1 > 0$, $(u^j)^T A u^{j+1} > 0$, $j = 1, \dots, n-1$. By Theorem 1 we then get that A is a copositive exceptional matrix. By Theorem 3 the matrix A is regular, which proves (i).

Consider the set $\mathcal{M} = \{X \in \mathcal{S}^n \mid \det X_{I_j} = 0 \ \forall\, j = 1, \dots, n\}$. It is defined by n polynomial equations, and $\hat{A} \in \mathcal{M}$. By virtue of Lemma 30 the gradient of the function $\det X_{I_j}$ at $X = \hat{A}$ is proportional to the rank 1 matrix $\hat{u}^j (\hat{u}^j)^T$. By Lemmas 15, 16, and Corollary 8 the linear span of the zeros $\hat{u}^j$ has dimension at least $n-1$. Since no two of these zeros are proportional, the gradients of the functions $\det X_{I_j}$ are linearly independent at $X = \hat{A}$ by Lemma 31. It follows that $\mathcal{M}$ is a smooth algebraic submanifold of codimension n in a neighbourhood of $\hat{A}$. This proves (ii). □

Theorem 5. *The extremal regular exceptional copositive matrices form an open subset of the manifold of all regular exceptional matrices.*

Proof. Assume the notations in the proof of the previous theorem, and suppose that $\hat{A}$ is extremal. The inequalities $(u^n)^T A u^1 > 0$, $(u^j)^T A u^{j+1} > 0$, $j = 1, \dots, n-1$ imply that the element $(Au^j)_i$ vanishes if and only if $i \in I_j$. Thus by Lemma 4 the matrix A is extremal if and only if the linear system of equations on the matrix $X \in \mathcal{S}^n$ given by

$$(Xu^j)_i = 0 \qquad \forall\, i \in I_j,\ j = 1, \dots, n \tag{13}$$

has a 1-dimensional solution space. The coefficients of this system depend linearly on the entries of the zeros u^j. Moreover, since $\hat{A}$ is extremal, system (13) has a 1-dimensional solution space for $u^j = \hat{u}^j$. But the rank of a matrix is a lower semi-continuous function, hence the solution space of (13) has dimension at most 1 if the zeros u^j are sufficiently close to $\hat{u}^j$. However, $X = A$ is always a solution, and therefore A is an extremal copositive matrix. □

The simplest manifold of the type described in Theorem 5 is the 10-dimensional union of the $\mathcal{G}_5$-orbits of the T-matrices (2). Matrices (2) themselves depend on 5 parameters, while the action of $\mathcal{G}_5$ adds another 5 parameters.

Theorem 6. *Let $n \geq 5$, and let $\hat{A} \in \mathcal{C}^n$ be a degenerate exceptional matrix having zeros $\hat{u}^1, \dots, \hat{u}^n \in \mathbb{R}^n_+$ such that $\operatorname{supp} \hat{u}^j = I_j$. Then there exists a neighbourhood $\mathcal{U} \subset \mathcal{S}^n$ of $\hat{A}$ with the following properties:*

(i) *if $A \in \mathcal{U}$ and $\operatorname{rk} A_{I_j} = n-4$ for all $j = 1, \dots, n$, then A is a degenerate exceptional extremal copositive matrix;*
(ii) *the set of matrices $A \in \mathcal{U}$ satisfying the conditions in (i) is an algebraic submanifold of codimension $2n$ in $\mathcal{S}^n$.*

Proof. By Theorem 3 the submatrices $\hat{A}_{I_j}$ have rank $n-4$ for $j = 1, \dots, n$. Let A be sufficiently close to $\hat{A}$ and suppose that $\operatorname{rk} A_{I_j} = n-4$ for all $j = 1, \dots, n$. By continuity the $n-4$ largest eigenvalues of A_{I_1} are then positive. However, the remaining two eigenvalues of A_{I_1} are zero by assumption, and hence $A_{I_1} \succeq 0$. Now the kernel of A_{I_1} is close to that of $\hat{A}_{I_1}$, hence $\ker A_{I_1}$ contains a positive vector close to $\hat{u}^1_{I_1}$. Then there exists a vector $u^1 \in \mathbb{R}^n_+$, close to $\hat{u}^1$, such that $\operatorname{supp} u^1 = I_1$ and $(u^1)^T A u^1 = 0$. In a similar way we construct vectors $u^j \in \mathbb{R}^n_+$, close to $\hat{u}^j$, such that $\operatorname{supp} u^j = I_j$ and $(u^j)^T A u^j = 0$, for all $j = 1, \dots, n$. By virtue of Theorem 1 we have $(\hat{u}^n)^T \hat{A} \hat{u}^1 > 0$ and $(\hat{u}^j)^T \hat{A} \hat{u}^{j+1} > 0$ for all $j = 1, \dots, n-1$. By continuity we then get $(u^n)^T A u^1 > 0$ and $(u^j)^T A u^{j+1} > 0$ for all $j = 1, \dots, n-1$. Again by Theorem 1 it then follows that A is an exceptional copositive matrix. By Theorem 3 the matrix A is also degenerate and extremal, which proves (i).

The proof of (ii) is a bit more complicated. Set $\hat{\mathbf{u}} = \{\hat{u}^1, \dots, \hat{u}^n\}$. By Lemma 13 we have $\hat{A} \in \mathcal{A}_{\hat{\mathbf{u}}}$. Let $\hat{B} = \Lambda(\hat{A})$ be the positive semi-definite symmetric bilinear form corresponding to $\hat{A}$.

By Corollary 3 each of the principal submatrices $\hat{A}_{I'_j}$ has a 1-dimensional kernel. For every $j = 1, \dots, n$, we define a vector $\hat{v}^j \in \mathbb{R}^n$ such that $\hat{v}^j_i = 0$ for all $i \notin I'_j$ and the subvector $\hat{v}^j_{I'_j}$ generates the kernel of $\hat{A}_{I'_j}$. We now claim the following:

(a) for every $j = 1, \dots, n-1$ we have $\ker \hat{A}_{I_j} = \operatorname{span}\{\hat{v}^j, \hat{v}^{j+1}\}$, and $\ker \hat{A}_{I_n} = \operatorname{span}\{\hat{v}^n, \hat{v}^1\}$;

(b) the first and the last element of the subvector $\hat{v}^j_{I'_j}$ is non-zero for all $j = 1, \dots, n$;

(c) the vectors $\hat{v}^1, \dots, \hat{v}^n$ are linearly independent.

Since the positive semi-definite quadratic form $\hat{A}_{I_2}$ vanishes on the subvectors $\hat{v}^2_{I_2}, \hat{v}^3_{I_2}$, we have that $\hat{v}^2_{I_2}, \hat{v}^3_{I_2} \in \ker \hat{A}_{I_2}$. Now $\dim \ker \hat{A}_{I_2} = 2$, and hence either $\ker \hat{A}_{I_2} = \operatorname{span}\{\hat{v}^2_{I_2}, \hat{v}^3_{I_2}\}$, or $\hat{v}^2, \hat{v}^3$ are linearly dependent.

Assume the latter for the sake of contradiction. Then the non-zero elements of $\hat{v}^2$ have indices in the intersection $I'_2 \cap I'_3 = \{3, \dots, n-2\}$. The relation $\hat{A}_{I_2} \hat{v}^2_{I_2} = 0$ together with (9) yields $\sum_{s=3}^{n-2} \hat{v}^2_s \hat{B}(\mathbf{e}_t, \mathbf{e}_s) = 0$ for all $t = 2, \dots, n-1$. The evaluation functionals $\mathbf{e}_2, \dots, \mathbf{e}_{n-1}$ span the whole space $\mathcal{L}^*_{\hat{\mathbf{u}}}$, and therefore we must have $\sum_{s=3}^{n-2} \hat{v}^2_s \hat{B}(\mathbf{e}_t, \mathbf{e}_s) = 0$ for all $t \geq 1$. In particular, we get $\sum_{s=3}^{n-2} \hat{v}^2_s \hat{B}(\mathbf{e}_t - \mathbf{e}_{t+n}, \mathbf{e}_s) = 0$ for all $t = 1, \dots, n-4$. Since $\hat{A}$ is exceptional, by virtue of Lemma 17 the coefficient matrix of this linear homogeneous system on the elements of $\hat{v}^2$ is regular. Therefore $\hat{v}^2 = 0$, leading to a contradiction.

It follows that $\ker \hat{A}_{I_2} = \operatorname{span}\{\hat{v}^2_{I_2}, \hat{v}^3_{I_2}\}$, and by repeating the argument after circular shifts of the indices we obtain (a). Since $\hat{u}^1 \in \ker \hat{A}_{I_1}$, we have $\hat{u}^1 = \alpha \hat{v}^1 + \beta \hat{v}^2$ for some coefficients α, β. In particular, we have $\hat{u}^1_1 = \alpha \hat{v}^1_1 > 0$, implying $\hat{v}^1_1 \neq 0$. Similarly, $\hat{u}^1_{n-2} = \beta \hat{v}^2_{n-2} > 0$ implies $\hat{v}^2_{n-2} \neq 0$. Repeating the argument after circular shifts of the indices we obtain (b).

Finally, let $w \in \mathbb{R}^n$ be such that $\langle \hat{v}^j, w \rangle = 0$ for all $j = 1, \dots, n$. By (a) and by Lemma 22 we have that every zero of $\hat{A}$ is a linear combination of the vectors $\hat{v}^j$. It follows that w is orthogonal to all zeros of $\hat{A}$. By Lemma 5 there exists $\varepsilon > 0$ such that $\hat{A} - \varepsilon w w^T \in \mathcal{C}^n$. But by Theorem 3 $\hat{A}$ is extremal. Therefore we must have $w = 0$, which yields (c).

We now prove (ii). Consider the set

$$\mathcal{M} = \left\{ X \in \mathcal{S}^n \;\middle|\; \begin{array}{l} \det X_{I'_j} = 0 \quad \forall j = 1, \dots, n; \\ \det(X_{ik})_{i \in I'_j; k \in I'_{j+1}} = 0 \quad \forall j = 1, \dots, n-1; \ \det(X_{ik})_{i \in I'_n; k \in I'_1} = 0 \end{array} \right\}.$$

It is defined by $2n$ polynomial equations, and $\hat{A} \in \mathcal{M}$. By Lemma 32 in a neighbourhood of $\hat{A}$ the manifold $\mathcal{M}$ coincides with the set of matrices A satisfying condition (i).

Now by virtue of Lemma 30 the gradient of the function $\det X_{I'_j}$ at $X = \hat{A}$ is proportional to the rank 1 matrix $\hat{v}^j(\hat{v}^j)^T$, the gradient of $\det(X_{ik})_{i\in I'_j;k\in I'_{j+1}}$ is proportional to the rank 1 matrix $\hat{v}^j(\hat{v}^{j+1})^T$, and the gradient of $\det(X_{ik})_{i\in I'_n;k\in I'_1}$ is proportional to $\hat{v}^n(\hat{v}^1)^T$. By (c) the vectors $\hat{v}^j$ are linearly independent, hence these $2n$ gradients are also linearly independent. It follows that $\mathcal{M}$ is a smooth algebraic submanifold of codimension $2n$ in a neighbourhood of $\hat{A}$. This proves (ii). □

The simplest manifold of the type described in Theorem 6 is the 5-dimensional $\mathcal{G}_5$-orbit of the Horn matrix (1).

7 Existence of non-trivial faces

So far we have always supposed that the feasible sets $\mathcal{F}_{\mathbf{u}}$ or $\mathcal{P}_{\mathbf{u}}$ of the LMIs in Theorem 2 contain non-zero forms. In this section we shall explicitly construct non-zero faces $\mathcal{F}_{\mathbf{u}}$ and $\mathcal{P}_{\mathbf{u}}$ for arbitrary matrix sizes $n \geq 5$.

7.1 Faces consisting of positive semi-definite matrices

In this subsection we construct non-zero faces $F_{\mathbf{u}}$ of $\mathcal{C}^n$ which contain only positive semi-definite matrices, i.e., which satisfy $F_{\mathbf{u}} = P_{\mathbf{u}}$.

We shall need the following concept of a *slack matrix*, which has been introduced in [20] for convex polytopes. Let $K \subset \mathbb{R}^m$ be a polyhedral convex cone, and let $K^* = \{f \in \mathbb{R}_m \mid \langle f, x\rangle \geq 0 \;\forall\, x \in K\}$ be its dual cone, where $\mathbb{R}_m$ is the space of linear functionals on $\mathbb{R}^m$. Then K^* is also a convex polyhedral cone. Let $x_1, \dots, x_r$ be generators of the extreme rays of K, and $f_1, \dots, f_s$ generators of the extreme rays of K^*.

Definition 3. Assume the notations of the previous paragraph. The *slack matrix* of K is the nonnegative $s \times r$ matrix $(\langle f_i, x_j\rangle)_{i=1,\dots,s;j=1,\dots,r}$.

Theorem 7. *Assume $n \geq 5$, and let $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}^n_+$ be such that $\operatorname{supp} u^j = I_j$ for all $j = 1, \dots, n$. Let U be the $n \times n$ matrix with columns $u^1, \dots, u^n$. Then the face $F_{\mathbf{u}}$ consists of positive semi-definite matrices up to rank $n-3$ inclusively if and only if U is the slack matrix of a convex polyhedral cone $K \subset \mathbb{R}^3$ with n extreme rays.*

Proof. By Theorem 2 and Lemma 19 we have $F_{\mathbf{u}} = P_{\mathbf{u}} \simeq \mathcal{S}_+^{n-3}$ if and only if $\operatorname{rk} U = 3$.

Assume $\operatorname{rk} U = 3$. Choose a factorization $U = U_L U_R^T$, with U_L, U_R being rank 3 matrices of size $n \times 3$. No two columns of U and hence no two rows of U_R are proportional, because $I_j \not\subset I_k$ for every $j \neq k$. Denote the convex conic hull of the rows of U_R by K. Row n of U_L is orthogonal to rows 1 and 2 of U_R and has a positive scalar product with the other rows of U_R. Therefore row n of U_L defines a supporting hyperplane to K, and the two-dimensional convex conic hull of row 1 and row 2 of U_R is a subset of the boundary of K. By a circular shift of the indices and by repeating the argument we extend the construction of the boundary of K until it closes in on itself. We obtain that K is a polyhedral cone with n extreme rays generated by the rows of U_R. On the other hand, the rows of U_L define exactly the supporting hyperplanes to K which intersect K in its two-dimensional faces. Therefore the dual cone

K^* is given by the convex conic hull of the rows of U_L. The relation $U = U_L U_R^T$ then reveals that U is the slack matrix of K.

On the other hand, a convex polyhedral cone $K \subset \mathbb{R}^3$ with $n \geq 3$ extreme rays as well as its dual K^* have a linear span of dimension 3. Therefore the slack matrix of such a cone has rank 3. This completes the proof. □

Theorem 7 provides a way to construct all collections $\mathbf{u} \subset \mathbb{R}_+^n$ of vectors $u^1, \dots, u^n$ with supports $\operatorname{supp} u^j = I_j$, $j = 1, \dots, n$, such that the face $F_\mathbf{u}$ of $\mathcal{C}^n$ consists of positive semi-definite matrices only and is linearly isomorphic to $\mathcal{S}_+^{n-3}$. By perturbing some of the zeros u^j in such a collection, we obtain faces $F_\mathbf{u}$ for which the subset $P_\mathbf{u}$ of positive semi-definite matrices is isomorphic to $\mathcal{S}_+^k$ with arbitrary rank $k = 0, \dots, n-3$. For $k \geq 2$ we have by Corollary 8 that $F_\mathbf{u} = P_\mathbf{u}$.

7.2 Circulant matrices

In this section we consider faces $F_\mathbf{u}$ defined by special collections $\mathbf{u}$. Let $u \in \mathbb{R}_+^{n-2}$ be *palindromic*, i.e., invariant with respect to inversion of the order of its entries, and with positive entries. Define $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}_+^n$ such that $\operatorname{supp} u^j = I_j$ and $u^j_{I_j} = u$ for all $j = 1, \dots, n$. By construction, the linear dynamical system $\mathbf{S_u}$ defined by $\mathbf{u}$ has constant coefficients, namely the entries of u. Let $p(x) = \sum_{k=0}^{n-3} u_{k+1} x^k$ be the characteristic polynomial of $\mathbf{S_u}$.

We provide necessary and sufficient conditions on $\mathbf{u}$ such that the corresponding face $F_\mathbf{u} \subset \mathcal{C}^n$ contains exceptional copositive matrices, and construct explicit collections $\mathbf{u}$ which satisfy these conditions. We show that the copositive matrices in these faces must be circulant, i.e., invariant with respect to simultaneous circular shifts of its row and column indices.

Lemma 23. *Suppose the collection $\mathbf{u}$ is as in the first paragraph of this section. If $F_\mathbf{u} \neq P_\mathbf{u}$, then $F_\mathbf{u}$ contains exceptional circulant matrices.*

Proof. Let $A^1 \in F_\mathbf{u}$ be exceptional. By simultaneous circular shifts of the row and column indices of A^1 we obtain copositive matrices $A^2, \dots, A^n$ which are also elements of $F_\mathbf{u}$. Then $A = \frac{1}{n} \sum_{j=1}^n A^j \in F_\mathbf{u}$ is a copositive circulant matrix. By Theorem 1 it is also exceptional. □

Lemma 24. *Suppose the collection $\mathbf{u}$ is as above, let $n \geq 5$, and let $A \in F_\mathbf{u}$ be a circulant matrix. Then the symmetric bilinear form $B = \Lambda(A)$ satisfies $B(\mathbf{e}_t, \mathbf{e}_s) = B(\mathbf{e}_{t+l}, \mathbf{e}_{s+l})$ for all $t, s, l \geq 1$.*

Proof. Define matrices $B_{r,l} = (B(\mathbf{e}_{r+t}, \mathbf{e}_{r+s}))_{t,s=0,\dots,l}$ of size $(l+1) \times (l+1)$, $r \geq 1$, $l \geq d$. By Lemma 10 for $l = d$ the matrices $B_{r,l}$ are equal to a single matrix B_l for all $r \geq 1$, and this matrix B_l is Toeplitz, rank-deficient, and has an element-wise positive kernel vector. We now show by induction that this holds also for all $l > d$.

Indeed, the entries of the positive semi-definite matrices $B_{r,l+1}$ are all determined by the matrix B_l, except the upper right (and lower left) corner element. Since B_l has a kernel vector with positive elements, Lemma 29 is applicable and these corner elements are unique and hence all equal for all $r \geq 1$. It follows that the matrices $B_{r,l+1}$ are all equal to a single matrix B_{l+1}. By construction this matrix is also Toeplitz and rank-deficient. Moreover, if $w \in \ker B_l$ is element-wise positive, then $(w^T, 0)^T + (0, w^T)^T \in \ker B_{l+1}$ is also element-wise positive.

The claim of the lemma now easily follows. □

Corollary 9. *Assume the conditions of the previous lemma and set* $r = \lfloor \frac{\operatorname{rk} B}{2} \rfloor$*. Then there exist distinct angles* $\varphi_0 = \pi$, $\varphi_1, \dots, \varphi_r \in (0, \pi)$ *and positive numbers* $\lambda_0, \dots, \lambda_r$ *such that*

$$B(\mathbf{e}_t, \mathbf{e}_s) = \begin{cases} \sum_{j=0}^r \lambda_j \cos(|t-s|\varphi_j), & \operatorname{rk} B \text{ odd}; \\ \sum_{j=1}^r \lambda_j \cos(|t-s|\varphi_j), & \operatorname{rk} B \text{ even} \end{cases}$$

for all $t, s \geq 1$*. Moreover,* $e^{\pm i\varphi_j}$ *are roots of* $p(x)$ *for all* $j = 1, \dots, r$*. In addition, if* $\operatorname{rk} B$ *is odd, then* -1 *is also a root of* $p(x)$*.*

Proof. By Theorem 2 we have $B \in \mathcal{F}_{\mathbf{u}}$. Hence the Toeplitz matrix $T = (B(\mathbf{e}_i, \mathbf{e}_j))_{i,j=1,\dots,n-2}$ is positive semi-definite, rank-deficient and of the same rank as B, and has the element-wise positive kernel vector u. The corollary follows by application of Lemma 33 to T and by Lemma 24. □

With the representation for $B(\mathbf{e}_t, \mathbf{e}_s)$ given by Corollary 9 relations (10) become

$$\begin{array}{lcll} \sum_{j=0}^r \lambda_j(\cos((n-k)\varphi_j) - \cos(k\varphi_j)) & = & 0, & \operatorname{rk} B \text{ odd}, \\ \sum_{j=1}^r \lambda_j(\cos((n-k)\varphi_j) - \cos(k\varphi_j)) & = & 0, & \operatorname{rk} B \text{ even}, \end{array} \quad 3 \leq k < \frac{n}{2}, \tag{14}$$

where k takes integer values, and inequalities (12) become

$$\begin{array}{lcll} \sum_{j=0}^r \lambda_j(\cos((n-2)\varphi_j) - \cos(2\varphi_j)) & \leq & 0, & \operatorname{rk} B \text{ odd}, \\ \sum_{j=1}^r \lambda_j(\cos((n-2)\varphi_j) - \cos(2\varphi_j)) & \leq & 0, & \operatorname{rk} B \text{ even}. \end{array} \tag{15}$$

Note that (14) is a linear homogeneous system of equations on the weights λ_j.

Lemma 25. *Let* $n > 5$ *be even, let* $\mathbf{u}$ *be as above, and let* $A \in F_{\mathbf{u}}$ *be an exceptional copositive circulant matrix. Then there exist* $m = \frac{n}{2} - 2$ *distinct angles* $\zeta_1, \dots, \zeta_m \in (0, \pi)$*, arranged in increasing order, with the following properties:*

(a) the fractional part of $\frac{n\zeta_j}{4\pi}$ *is in* $(0, \frac{1}{2})$ *for odd* j *and in* $(\frac{1}{2}, 1)$ *for even* j*;*

(b) the polynomial $p(x)$ *is proportional to the polynomial* $(x+1) \cdot \prod_{j=1}^m (x^2 - 2x\cos\zeta_j + 1)$*;*

(c) there exist $c > 0$*,* $\lambda \geq 0$ *such that for all* $k = 1, \dots, \frac{n}{2} + 1$ *we have*

$$A_{1k} = (-1)^{k-1}\lambda + c \cdot \sum_{j=1}^m \frac{\cos(k-1)\zeta_j}{\sin\zeta_j \sin\frac{n\zeta_j}{2} \prod_{l \neq j}(\cos\zeta_j - \cos\zeta_l)}. \tag{16}$$

If $\lambda = 0$*, then* A *is degenerate and extremal. If* $\lambda > 0$*, then* A *is regular and not extremal.*

Proof. Let $B = \Lambda(A)$ and apply Corollary 9. By Corollary 7 we have either $\operatorname{rk} B = n - 4$ or $\operatorname{rk} B = n - 3$ and hence $m = r$. Define $\zeta_1, \dots, \zeta_m$ to be the angles $\varphi_1, \dots, \varphi_r$, arranged in increasing order. Then $e^{\pm i\zeta_j}$ are roots of $p(x)$ by Corollary 9, and $p(x)$ is of the form $\alpha \cdot (x - \beta) \cdot \prod_{j=1}^m (x^2 - 2x\cos\zeta_j + 1)$ for some $\alpha > 0$ and real β. Since the coefficient vector u of $p(x)$ is palindromic, we must have $\beta = -1$, which proves (b).

By (9) we have $A_{1k} = B(\mathbf{e}_1, \mathbf{e}_k)$, $k = 1, \dots, \frac{n+1}{2}$, which in turn is given by Corollary 9. Here the weights λ_j satisfy relations (14),(15), the inequality being strict by Lemma 13. We have $\varphi_0 = \pi$ and hence $\cos((n-k)\varphi_0) = \cos(k\varphi_0)$ for all integers k. Therefore (14),(15) do not impose any conditions on the coefficient λ_0, and these m relations can be considered as conditions on $\lambda_1, \dots, \lambda_m$ only. By Corollary 10 there are no multiples of $\frac{2\pi}{n}$ among the angles $\zeta_1, \dots, \zeta_m$, and the coefficient vector

$(\lambda_1, \dots, \lambda_m)$ is proportional to solution (27) in this corollary. This yields (c) with $c > 0$, with $\lambda = 0$ if $\operatorname{rk} B = n - 4$, and with $\lambda = \lambda_0 > 0$ if $\operatorname{rk} B = n - 3$.

The last assertions of the lemma now follow from Theorem 3.

Finally, the weights $\lambda_1, \dots, \lambda_m$ are positive by Corollary 9, and their explicit expression from Corollary 10 yields $\sin \zeta_j \sin \frac{n\zeta_j}{2} \prod_{l \neq j}(\cos \zeta_j - \cos \zeta_l) > 0$. Since the cosine function is strictly decreasing on $(0, \pi)$ and the ζ_j are arranged in increasing order, it follows that $\operatorname{sgn} \sin \frac{n\zeta_j}{2} = \operatorname{sgn} \prod_{l \neq j}(\cos \zeta_j - \cos \zeta_l) = (-1)^{j+1}$, which implies (a). □

Lemma 26. *Let $n \geq 5$ be odd, let $\mathbf{u}$ be as above, and let $A \in F_{\mathbf{u}}$ be an exceptional copositive circulant matrix. Then there exist $m = \frac{n-3}{2}$ distinct angles $\zeta_1, \dots, \zeta_m \in (0, \pi]$, arranged in increasing order, with the following properties:*

(a) the fractional part of $\frac{n\zeta_j}{4\pi}$ is in $(0, \frac{1}{2})$ for odd j and in $(\frac{1}{2}, 1)$ for even j;

(b) the polynomial $p(x)$ is proportional to the polynomial $\prod_{j=1}^{m}(x^2 - 2x \cos \zeta_j + 1)$;

(c) there exists $c > 0$ such that for all $k = 1, \dots, \frac{n+1}{2}$ we have

$$A_{1k} = c \cdot \sum_{j=1}^{m} \frac{\cos(k-1)\zeta_j}{\sin \frac{\zeta_j}{2} \sin \frac{n\zeta_j}{2} \prod_{l \neq j}(\cos \zeta_j - \cos \zeta_l)}. \tag{17}$$

The matrix A is degenerate if $\zeta_m = \pi$ and regular if $\zeta_m < \pi$. In both cases A is extremal.

Proof. Let $B = \Lambda(A)$ and apply Corollary 9. By Corollary 7 we have either $\operatorname{rk} B = n - 4$ or $\operatorname{rk} B = n - 3$, which gives $m = r + 1$ or $m = r$, respectively. Define $\zeta_1, \dots, \zeta_m$ to be the angles $\varphi_0, \dots, \varphi_r$ in the first case and $\varphi_1, \dots, \varphi_r$ in the second case, arranged in increasing order. Then $\zeta_m = \pi$ if $\operatorname{rk} B = n - 4$ and $\zeta_m < \pi$ if $\operatorname{rk} B = n - 3$. By Corollary 9 the numbers $e^{\pm i\zeta_j}$ are roots of $p(x)$, and $p(x)$ is of the form $\alpha \cdot (x + 1) \cdot (x - \beta) \cdot \prod_{j=1}^{m-1}(x^2 - 2x \cos \zeta_j + 1)$ if $\zeta_m = \pi$ and $p(x) = \alpha \cdot \prod_{j=1}^{m}(x^2 - 2x \cos \zeta_j + 1)$ if $\zeta_m < \pi$, for some $\alpha > 0$ and real β. Since the coefficient vector u of $p(x)$ is palindromic, we must have $\beta = -1$, which proves (b).

By Theorem 3 the matrix A is degenerate and extremal if $\zeta_m = \pi$, and regular if $\zeta_m < \pi$.

By (9) we have $A_{1k} = B(\mathbf{e}_1, \mathbf{e}_k)$, $k = 1, \dots, \frac{n+1}{2}$, which in turn is given by Corollary 9. Here the m coefficients λ_j satisfy the m relations (14),(15), the inequality being strict by Lemma 13. By Corollary 10 there are no multiples of $\frac{2\pi}{n}$ among the angles $\zeta_1, \dots, \zeta_m$, and the coefficient vector $(\lambda_1, \dots, \lambda_m)$ is proportional to solution (27) in this corollary. This yields (c) with $c > 0$.

Assertion (a) is obtained in the same way as in the proof of Lemma 25.

It remains to show the extremality of A for $\zeta_m < \pi$. By Lemma 38 in Appendix B the dimension of the space $\mathcal{A}_{\mathbf{u}}$ cannot exceed 1, otherwise we obtain a contradiction with the nonnegativity of u. It follows that $\dim F_{\mathbf{u}} = 1$ and A is extremal in $\mathcal{C}^n$. □

Note that the elements A_{1k}, $k = 1, \dots, \lceil \frac{n+1}{2} \rceil$, determine the matrix A completely by its circulant property. We obtain the following characterization of collections $\mathbf{u}$ defining faces $F_{\mathbf{u}}$ which contain exceptional matrices.

Theorem 8. *Let $n > 5$ be even, $m = \frac{n}{2} - 2$, and let $\mathbf{u}$ and $p(x)$ be as in the first paragraph of this section. Then $F_{\mathbf{u}} \neq P_{\mathbf{u}}$ if and only if there exist distinct angles $\zeta_1, \dots, \zeta_m \in (0, \pi)$, arranged in increasing order, such that conditions (a),(b) of Lemma 25 hold. In this case the face $F_{\mathbf{u}}$ is linearly* *isomorphic to* $\mathbb{R}_+^2$ *and consists of the circulant matrices* A *with entries* A_{1k}*,* $k = 1, \dots, \frac{n}{2} + 1$*, given by* (16) *with* $c, \lambda \geq 0$*. The subset* $P_{\mathbf{u}} \subset F_{\mathbf{u}}$ *is given by those* A *with* $c = 0$*.*

Proof. Suppose $F_{\mathbf{u}} \neq P_{\mathbf{u}}$. Then by Lemma 23 there exists a circulant matrix $A \in F_{\mathbf{u}} \setminus P_{\mathbf{u}}$. Hence Lemma 25 applies and conditions (a),(b) hold.

Let now $\zeta_1, \dots, \zeta_m \in (0, \pi)$ be an increasing sequence of angles satisfying conditions (a),(b) of Lemma 25. Define weights $\lambda_1, \dots, \lambda_m$ by (27). By condition (a) these weights are positive, and by Corollary 10 they satisfy system (26). Let $A \in \mathcal{S}^n$ be the circulant matrix satisfying $A_{1k} = \sum_{j=1}^m \lambda_j \cos(k-1)\zeta_j$ for $k = 1, \dots, \frac{n}{2} + 1$. By (26) the last relation actually holds for $k = 1, \dots, n-2$, and $A_{1,n-1} > \sum_{j=1}^m \lambda_j \cos(n-2)\zeta_j$. By construction the submatrices A_{I_j} are positive semi-definite of rank $2m = n - 4$ and by condition (b) they possess the kernel vector $u = u^j_{I_j}$. Moreover, the preceding inequality implies that $(u^n)^T A u^1 > 0$ and $(u^j)^T A u^{j+1} > 0$ for $j = 1, \dots, n-1$. By Theorem 1 we then have $A \in F_{\mathbf{u}} \setminus P_{\mathbf{u}}$, proving the equivalence claimed in the theorem.

Let $P \in \mathcal{S}_+^n$ be the positive semi-definite circulant rank 1 matrix given element-wise by $P_{kl} = (-1)^{k-l}$. Since the subvectors $u^j_{I_j}$ are palindromic and have an even number of entries, we get that $(u^j)^T P u^j = 0$ for all $j = 1, \dots, n$. Hence $P \in P_{\mathbf{u}}$ and $r_{PSD} \geq 1$, where r_{PSD} is the maximal rank achieved by matrices in $P_{\mathbf{u}}$. But then $r_{PSD} = 1$ and $r_{\max} = n - 3$ by Corollary 8, and the last assertion of the theorem follows.

By Lemma 20 we have $F_{\mathbf{u}} \simeq \mathbb{R}_+^2$. However, the matrices A and P constructed above are linearly independent elements of $F_{\mathbf{u}}$, and therefore $F_{\mathbf{u}} \subset \mathrm{span}\{A, P\}$ consists of circulant matrices only. The remaining assertions now follow from Lemma 25. □

Theorem 9. *Let* $n \geq 5$ *be odd,* $m = \frac{n-3}{2}$*, and let* $\mathbf{u}$ *and* $p(x)$ *be as in the first paragraph of this section. Then* $F_{\mathbf{u}} \neq P_{\mathbf{u}}$ *if and only if there exist distinct angles* $\zeta_1, \dots, \zeta_m \in (0, \pi]$*, arranged in increasing order, such that conditions (a),(b) of Lemma 26 hold. In this case the face* $F_{\mathbf{u}}$ *is an extreme ray of* $\mathcal{C}^n$ *and consists of the circulant matrices* A *with entries* A_{1k}*,* $k = 1, \dots, \frac{n+1}{2}$*, given by* (17) *with* $c \geq 0$*.*

Proof. The proof of the theorem is similar to the proof of Theorem 8, with obvious modifications. □

The question which collections $\mathbf{u}$, of the type described at the beginning of this subsection, yield faces $F_{\mathbf{u}}$ containing exceptional copositive matrices hence reduces to the characterization of real polynomials of the form given in (b) of Lemmas 25 or 26, with positive coefficients and satisfying condition (a) of these lemmas. This is seemingly a difficult question, and only limited results are known. However, the existence of faces $F_{\mathbf{u}}$ containing exceptional copositive matrices is guaranteed for every $n \geq 5$ by the following result on polynomials with equally spaced roots on the unit circle.

Lemma 27. *[12, Theorem 2] Let* $m \geq 1$ *be an integer, and let* $\alpha > 0$*,* $\theta \geq 0$ *be such that* $\frac{\pi}{2} \leq \theta + \frac{(m-1)\alpha}{2} \leq \pi$ *and* $0 < \alpha < \frac{\pi}{m}$*. Then the polynomial* $q(x) = \prod_{j=1}^m (x^2 - 2x\cos(\theta + (j-1)\alpha) + 1)$ *has positive coefficients.*

Indeed, the lemma allows to construct the following explicit examples.

Degenerate extremal matrices. Let $n \geq 5$, $m = \lceil \frac{n}{2} \rceil - 2$, and $p(x) = \frac{(x^n+1)(x+1)}{(x^2-2x\cos\frac{\pi}{n}+1)(x^2-2x\cos\frac{3\pi}{n}+1)}$. Then $p(x)$ is a palindromic polynomial of degree $n-3$. Set also $q(x) = p(x)$ for odd n and $q(x) = \frac{p(x)}{x+1}$ for even n. Then $q(x)$ is of degree $2m$ and has positive coefficients by virtue of Lemma 27 with $\alpha = \frac{2\pi}{n}$,

$\theta = \frac{5\pi}{n}$. It follows that also $p(x)$ has positive coefficients. Let $u \in \mathbb{R}_+^{n-2}$ be the vector of its coefficients, and let $\mathbf{u}$ be the collection of nonnegative vectors constructed from u as in the first paragraph of this section. Then the angles $\zeta_j = \frac{(2j+3)\pi}{n}$, $j = 1, \dots, m$, satisfy conditions (a),(b) of Lemmas 25 and 26, for even and odd n, respectively. By Theorems 8 and 9 we obtain that $F_{\mathbf{u}} \simeq \mathbb{R}_+^2$ for even n and $F_{\mathbf{u}} \simeq \mathbb{R}_+$ for odd n, their elements being circulant matrices given by (16) and (17), respectively. One extreme ray of $F_{\mathbf{u}}$ is then generated by an extremal degenerate copositive circulant matrix A. For even n the other extreme ray is generated by a circulant positive semi-definite rank 1 matrix P. Their elements are given by $P_{ij} = (-1)^{i-j}$ and

$$A_{ij} = \begin{cases} 2(1 + 2\cos\frac{\pi}{n}\cos\frac{3\pi}{n}), & i = j, \\ -2(\cos\frac{\pi}{n} + \cos\frac{3\pi}{n}), & |i-j| \in \{1, n-1\}, \\ 1, & |i-j| \in \{2, n-2\}, \\ 0, & |i-j| \in \{3, \dots, n-3\}, \end{cases} \quad (18)$$

$i, j = 1, \dots, n.$

Regular extremal matrices. Let $n \geq 5$ be odd, and set $m = \frac{n-3}{2}$. Then the polynomial $p(x) = \frac{x^{n+1}+1}{(x^2-2x\cos\frac{\pi}{n+1}+1)(x^2-2x\cos\frac{3\pi}{n+1}+1)}$ is palindromic of degree $2m = n-3$, and it has positive coefficients by virtue of Lemma 27 with $\alpha = \frac{2\pi}{n+1}$, $\theta = \frac{5\pi}{n+1}$. Construct $u \in \mathbb{R}_+^{n-2}$ and $\mathbf{u} \subset \mathbb{R}_+^n$ as above from the coefficients of $p(x)$. Then the angles $\zeta_j = \frac{(2j+3)\pi}{n+1}$, $j = 1, \dots, m$, satisfy conditions (a),(b) of Lemma 26. By Theorem 9 $F_{\mathbf{u}}$ is one-dimensional and generated by a circulant regular extremal copositive matrix whose elements are given by (17). Explicitly this gives

$$A_{ij} = \begin{cases} 2(1 + 2\cos\frac{\pi}{n+1}\cos\frac{3\pi}{n+1}), & i = j, \\ -2(\cos\frac{\pi}{n+1} + \cos\frac{3\pi}{n+1}), & |i-j| \in \{1, n-1\}, \\ 1, & |i-j| \in \{2, n-2\}, \\ 0, & |i-j| \in \{3, \dots, n-3\}, \end{cases} \quad (19)$$

$i, j = 1, \dots, n.$

However, Lemma 27 allows also for other choices of regularly spaced angles $\zeta_1, \dots, \zeta_m$ or regularly spaced angles $\zeta_1, \dots, \zeta_{m-1}, 2\pi - \zeta_m$. The following result guarantees the positivity of the coefficients of $p(x)$ also in the case when only $\zeta_2, \dots, \zeta_m$ (or $\zeta_2, \dots, \zeta_{m-1}, 2\pi - \zeta_m$) are regularly spaced, and the spacing between ζ_1 and ζ_2 is inferior to the spacing between the other angles.

Lemma 28. *[1, Corollary 1.1] Let $p(x)$ be a real polynomial with nonnegative coefficients, and let x_0 be the root of $p(x)$ which has the smallest argument among all roots of $p(x)$ in the upper half-plane. If x_1 is any number such that $|x_1| \geq |x_0|$ and $Re\, x_1 \leq Re\, x_0$, then the coefficients of the polynomial $p(x)\frac{(x-x_1)(x-\bar{x}_1)}{(x-x_0)(x-\bar{x}_0)}$ are not smaller than the corresponding coefficients of $p(x)$.*

As to the general case, we establish the following conjecture.

Conjecture 1. *Let $n \geq 5$ be an integer, and set $m = \lceil \frac{n}{2} \rceil - 2$. Let $\zeta_1, \dots, \zeta_m \in (0, \pi]$ be an increasing sequence of angles such that the fractional part of $\frac{n\zeta_j}{4\pi}$ is in $(0, \frac{1}{2})$ for odd j and in $(\frac{1}{2}, 1)$ for even j. Define the polynomial $q(x) = \prod_{j=1}^m (x^2 - 2x\cos\zeta_j + 1)$, and set $p(x) = q(x)$ for odd n and $p(x) = (x+1)q(x)$ for even n. Then the coefficients of $p(x)$ are all positive if and only if $\zeta_j \in (\frac{(2j+2)\pi}{n}, \frac{(2j+4)\pi}{n})$ for all $j = 1, \dots, m$.*

We have verified this conjecture for $n \leq 8$.

8 Matrices of order 6

In this section we compute all exceptional extremal copositive matrices A of size 6×6 which have zeros u^j with $\operatorname{supp} u^j = I_j$, $j = 1, \dots, 6$. We assume without loss of generality that $\operatorname{diag} A = (1, \dots, 1)$, because every other such matrix lies in the $\mathcal{G}_6$-orbit of a matrix normalized in this way.

Let $A \in \mathcal{C}^6$ be exceptional and extremal, $\operatorname{diag} A = (1, \dots, 1)$, and let $\mathbf{u} = \{u^1, \dots, u^6\} \subset \mathbb{R}^6_+$ be zeros of A satisfying $\operatorname{supp} u^j = I_j$. By Theorem 3 the matrix A is degenerate, and $\operatorname{rk} A_{I_j} = 2$ for all $j = 1, \dots, 6$. Therefore $B = \Lambda(A)$ has rank 2 by Corollary 3, and $B = x \otimes x + y \otimes y$ for some solutions $x = (x_1, x_2, \dots), y = (y_1, y_2, \dots) \in \mathcal{L}_\mathbf{u}$. Extremality of A implies that the linear span of $\{x, y\}$ does not contain non-zero periodic solutions. Indeed, let $v \in \operatorname{span}\{x, y\}$ be such a solution. Then $v \otimes v \in \mathcal{P}_\mathbf{u}$, and $B \pm \varepsilon \cdot v \otimes v \in \mathcal{F}_\mathbf{u}$ for ε small enough. Hence A can be represented as a non-trivial convex combination of the elements $\Lambda^{-1}(B \pm \varepsilon v \otimes v) \in F_\mathbf{u}$, contradicting extremality.

Shift-invariance of B implies that the monodromy $\mathfrak{M}$ of the system $\mathbf{S}_\mathbf{u}$ acts on $x, y \in \mathcal{L}_\mathbf{u}$ by

$$\begin{pmatrix} \mathfrak{M}x \\ \mathfrak{M}y \end{pmatrix} = M \begin{pmatrix} x \\ y \end{pmatrix},$$

where M is an orthogonal 2×2 matrix. If M is a reflection, then $\mathfrak{M}$ has an eigenvector with eigenvalue 1 in the span of $\{x, y\}$, leading to a contradiction by Lemma 6. Hence M is a rotation by an angle $\zeta \in (0, 2\pi)$, i.e.,

$$\mathfrak{M}x = \cos\zeta \cdot x - \sin\zeta \cdot y, \qquad \mathfrak{M}y = \sin\zeta \cdot x + \cos\zeta \cdot y. \tag{20}$$

By (9) and by the normalization adopted above we have $x_k^2 + y_k^2 = 1$ for all $k \geq 1$. Without loss of generality we may assume that $x_1 = 1$, $y_1 = 0$, otherwise we rotate the basis $\{x, y\}$ of $\operatorname{span}\{x, y\}$ appropriately by redefining x, y. Then we have

$$x_k = \cos \sum_{j=1}^{k-1} (\pi - \varphi_j), \qquad y_k = \sin \sum_{j=1}^{k-1} (\pi - \varphi_j)$$

for some angles $\varphi_1, \varphi_2, \dots \in [0, 2\pi)$, for all $k \geq 1$. By virtue of (20) we get

$$\sum_{j=k}^{k+5} (\pi - \varphi_j) \equiv -\sum_{j=k}^{k+5} \varphi_j \equiv \zeta \mod 2\pi \qquad \forall\, k \geq 1.$$

It follows that $\varphi_k \equiv \varphi_{k+6}$ modulo 2π for all $k \geq 1$, and the sequence $\{\varphi_k\}$ is 6-periodic.

We have

$$B(\mathbf{e}_t, \mathbf{e}_s) = x_t x_s + y_t y_s = (-1)^{s-t} \cos \sum_{j=\min(t,s)}^{\max(t,s)-1} \varphi_j, \qquad \forall\, t, s \geq 1. \tag{21}$$

Conditions (10) reduce to $B(\mathbf{e}_t, \mathbf{e}_{t+3}) = B(\mathbf{e}_{t+3}, \mathbf{e}_{t+6})$ for all $t \geq 1$, which yields

$$\cos(\varphi_t + \varphi_{t+1} + \varphi_{t+2}) = \cos(\varphi_{t+3} + \varphi_{t+4} + \varphi_{t+5}) = \cos(\zeta + \varphi_t + \varphi_{t+1} + \varphi_{t+2}) \qquad \forall\, t \geq 1. \tag{22}$$

By virtue of $\zeta \neq 0$ it follows that $\varphi_t + \varphi_{t+1} + \varphi_{t+2} \equiv -(\zeta + \varphi_t + \varphi_{t+1} + \varphi_{t+2})$ modulo 2π, or equivalently,

$$\varphi_t + \varphi_{t+1} + \varphi_{t+2} \equiv -\frac{\zeta}{2} \mod \pi \qquad \forall\, t \geq 1.$$

This yields $\varphi_t \equiv \varphi_{t+3}$ modulo π, or $\varphi_{t+3} = \varphi_t + \delta_t$ with $\delta_t \in \{-\pi, 0, \pi\}$, for all $t \geq 1$.

By Lemma 13 inequalities (12) hold strictly, which yields

$$\cos(\varphi_t + \varphi_{t+1}) > \cos(\varphi_{t+2} + \varphi_{t+3} + \varphi_{t+4} + \varphi_{t+5}) = \cos(\zeta + \varphi_t + \varphi_{t+1}) \qquad \forall\, t \geq 1. \quad (23)$$

Equivalently, $\varphi_t + \varphi_{t+1} \in 2\pi l_t + (-\frac{\zeta}{2}, \pi - \frac{\zeta}{2})$ for some $l_t \in \{0, 1, 2\}$, for all $t \geq 1$. Replacing t by $t+3$, we get $\varphi_{t+3} + \varphi_{t+4} = \varphi_t + \varphi_{t+1} + \delta_t + \delta_{t+1} \in 2\pi l_{t+3} + (-\frac{\zeta}{2}, \pi - \frac{\zeta}{2})$, and therefore $\delta_t + \delta_{t+1} \equiv 0$ modulo 2π, for all $t \geq 1$. It follows that either $\delta_t = 0$ for all t, or $\delta_t \in \{-\pi, \pi\}$ for all t.

Assume the second case, for the sake of contradiction. Then $\cos(\varphi_{t+3} + \varphi_{t+4} + \varphi_{t+5}) = -\cos(\varphi_t + \varphi_{t+1} + \varphi_{t+2})$, which together with (22) gives $\varphi_t + \varphi_{t+1} + \varphi_{t+2} \equiv \frac{\pi}{2}$ modulo π for all $t \geq 1$, and $\zeta = \pi$. Inequality (23) yields $\cos(\varphi_t + \varphi_{t+1}) > 0$ for all $t \geq 1$. We then get $x_1 = 1$, $x_3 > 0$, $x_4 = 0$. But x is the solution of a 3-rd order linear system with positive coefficients. Hence $x_2 < 0$, and $\varphi_1 \notin [\frac{\pi}{2}, \frac{3\pi}{2}]$. By a similar argument, this has to be true for all φ_t, $t \geq 1$, contradicting $\delta_t \in \{-\pi, \pi\}$.

Therefore $\varphi_{t+3} = \varphi_t$ for all $t \geq 1$. Set $\sigma = \varphi_1 + \varphi_2 + \varphi_3$. Then (23) reduces to $\cos(\sigma - \varphi_j) > \cos(\sigma + \varphi_j)$, or equivalently $\sin\sigma \sin\varphi_j > 0$ for $j = 1, 2, 3$. Therefore $\sin\varphi_j$ and $\sin\sigma$ have the same sign for all $j = 1, 2, 3$. By possibly replacing the solution y by $-y$, we may assume without loss of generality that $\sin\varphi_1 > 0$ and hence $\varphi_j \in (0, \pi)$, $\pi - \varphi_j \in (0, \pi)$ for all $j = 1, 2, 3$. If $\sigma \in (2\pi, 3\pi)$, then $\sum_{j=1}^3 (\pi - \varphi_j) \in (0, \pi)$, and $y_k > 0$ for $k = 2, 3, 4$. Since also $y_1 = 0$, this contradicts the condition that y is a solution of a linear 3-rd order system with positive coefficients. Therefore $\varphi_1 + \varphi_2 + \varphi_3 < \pi$. By (9),(21) the matrix A is then given by

$$\begin{pmatrix} 1 & -\cos\varphi_1 & \cos(\varphi_1+\varphi_2) & -\cos(\varphi_1+\varphi_2+\varphi_3) & \cos(\varphi_2+\varphi_3) & -\cos\varphi_3 \\ -\cos\varphi_1 & 1 & -\cos\varphi_2 & \cos(\varphi_2+\varphi_3) & -\cos(\varphi_1+\varphi_2+\varphi_3) & \cos(\varphi_1+\varphi_3) \\ \cos(\varphi_1+\varphi_2) & -\cos\varphi_2 & 1 & -\cos\varphi_3 & \cos(\varphi_1+\varphi_3) & -\cos(\varphi_1+\varphi_2+\varphi_3) \\ -\cos(\varphi_1+\varphi_2+\varphi_3) & \cos(\varphi_2+\varphi_3) & -\cos\varphi_3 & 1 & -\cos\varphi_1 & \cos(\varphi_1+\varphi_2) \\ \cos(\varphi_2+\varphi_3) & -\cos(\varphi_1+\varphi_2+\varphi_3) & \cos(\varphi_1+\varphi_3) & -\cos\varphi_1 & 1 & -\cos\varphi_2 \\ -\cos\varphi_3 & \cos(\varphi_1+\varphi_3) & -\cos(\varphi_1+\varphi_2+\varphi_3) & \cos(\varphi_1+\varphi_2) & -\cos\varphi_2 & 1 \end{pmatrix}. \quad (24)$$

On the other hand, let $\varphi_1, \varphi_2, \varphi_3 > 0$ such that $\varphi_1 + \varphi_2 + \varphi_3 < \pi$, and consider the matrix A given by (24). Let $v^1, \dots, v^6 \in \mathbb{R}^6_+$ be the columns of the matrix

$$V = \begin{pmatrix} \sin\varphi_2 & 0 & 0 & 0 & \sin\varphi_2 & \sin(\varphi_1+\varphi_3) \\ \sin(\varphi_1+\varphi_2) & \sin\varphi_3 & 0 & 0 & 0 & \sin\varphi_3 \\ \sin\varphi_1 & \sin(\varphi_2+\varphi_3) & \sin\varphi_1 & 0 & 0 & 0 \\ 0 & \sin\varphi_2 & \sin(\varphi_1+\varphi_3) & \sin\varphi_2 & 0 & 0 \\ 0 & 0 & \sin\varphi_3 & \sin(\varphi_1+\varphi_2) & \sin\varphi_3 & 0 \\ 0 & 0 & 0 & \sin\varphi_1 & \sin(\varphi_2+\varphi_3) & \sin\varphi_1 \end{pmatrix}, \quad (25)$$

and define $u^j = v^j + v^{j+1}$, $j = 1, \dots, 5$, $u^6 = v^6 + v^1$. By construction the submatrices A_{I_j} are positive semi-definite and of rank 2, and $(u^j)^T A u^j = 0$, $\operatorname{supp} u^j = I_j$ for all $j = 1, \dots, 6$. Moreover, $(u^j)^T A u^{j+1} > 0$ for all $j = 1, \dots, 5$ and $(u^6)^T A u^1 > 0$. Hence A is an exceptional copositive matrix by Theorem 1, and it is degenerate and extremal by Theorem 3. By (ii.d) of Theorem 3 the columns of V are minimal zeros of A, and every minimal zero of A is a positive multiple of some column of V. We have proven the following result.

Theorem 10. *Let $A \in \mathcal{C}^6$ be exceptional and extremal with zeros $u^1, \dots, u^n$ satisfying $\operatorname{supp} u^j = I_j$ for all $j = 1, \dots, 6$. Then A is in the $\mathcal{G}_6$-orbit of some matrix of the form* (24)*, with $\varphi_1, \varphi_2, \varphi_3 > 0$ and $\varphi_1 + \varphi_2 + \varphi_3 < \pi$. The minimal zero pattern of A is given by*

$\{\{1,2,3\},\{2,3,4\},\{3,4,5\},\{4,5,6\},\{1,5,6\},\{1,2,6\}\}$. *On the other hand, every matrix A of the form* (24) *with $\varphi_1,\varphi_2,\varphi_3 > 0$ and $\varphi_1+\varphi_2+\varphi_3 < \pi$ is exceptional and extremal, and every minimal zero of A is proportional to one of the columns of the matrix* (25). □

Remark 1. We do not claim that every extremal exceptional copositive matrix in $\mathcal{C}^6$ with $\operatorname{diag} A = (1,\dots,1)$ and with this minimal zero pattern has to be of the form (24).

9 Conclusions

In this contribution we considered copositive matrices with zeros $u^1,\dots,u^n \in \mathbb{R}^n_+$ having supports $\operatorname{supp} u^j = I_j$. Exceptional copositive matrices with this property exist for all matrix sizes $n \geq 5$ and are of two types, in dependence on whether the zeros u^j are minimal or not. The matrices of each type make up an algebraic submanifold of $\mathcal{S}^n$, of codimensions n and $2n$, respectively. The prototypes of these matrices are the T-matrices and the Horn matrix, respectively. Explicit examples of such matrices have been given in (19) and (18), respectively. We show that if the zeros u^j are not minimal, then the corresponding exceptional copositive matrices are extremal. If the zeros u^j are minimal, then the corresponding matrices can be extremal only for odd n.

Some open questions within this framework remain:

- Do regular non-extremal matrices exist for odd matrix size?
- Do degenerate matrices with minimal zero pattern different from $\{I'_1,\dots,I'_n\}$ exist?
- Which types of extremal copositive matrices can appear on the boundary of the submanifolds of regular and degenerate matrices, respectively?
- What is the global topology of these submanifolds?

A Auxiliary results

In this section we collect a few auxiliary results of general nature.

Lemma 29. *Let $A \in \mathcal{S}^n$ and define the ordered index subsets $I = (1,\dots,n-1)$, $I' = (2,\dots,n)$. Suppose that the principal submatrices $A_I, A_{I'}$ are positive semi-definite, and that there exist vectors $u,v \in \mathbb{R}^n$ such that $u_1, v_n > 0$, $v_1 = u_n = 0$, and $u^TAu = v^TAv = 0$. Then there exists a unique real number δ such that $A - \delta \cdot E_{1n}$ is positive semi-definite, and this number has the same sign as the product u^TAv.*

Proof. Consider the matrix-valued function $P(\delta) = A - \delta E_{1n}$. All elements of $P(\delta)$ except the upper right (and correspondingly lower left) corner element coincide with the corresponding elements of A. Therefore the posed problem on the unknown δ can be considered as a positive semi-definite matrix completion problem. Namely, we wish to modify the corner elements of A to make it positive semi-definite. By a standard result on positive semi-definite matrix completions [13] there exists a solution δ such that $P(\delta) \succeq 0$.

On the other hand, for every solution δ we have $u^TP(\delta)u = v^TP(\delta)v = 0$ and therefore must have $u^TP(\delta)v = 0$. Uniqueness of the solution follows and we have the explicit expression $\delta = \frac{u^TAv}{u^TE_{1n}v}$. The assertion of the lemma now follows from the strict inequality $u^TE_{1n}v > 0$. □

Lemma 30. *Define the set $\mathcal{M} = \{M \in \mathbb{R}^{n\times n} \mid \det M = 0\}$, and let $M \in \mathcal{M}$ be a matrix of corank 1. Let the vectors $u, v \in \mathbb{R}^n$ be generators of the left and the right kernel of M, respectively. Then the orthogonal complement under the Frobenius scalar product $\langle A, B\rangle = \mathrm{tr}(AB^T)$ of the tangent space to $\mathcal{M}$ at M is generated by the rank 1 matrix uv^T.*

Proof. Let $M = F_L^0(F_R^0)^T$ be a factorization of M, where F_L^0, F_R^0 are full column rank $n \times (n-1)$ matrices. The set $\mathcal{M}$ can be written as $\{F_L F_R^T \mid F_L, F_R \in \mathbb{R}^{n\times(n-1)}\}$. Therefore the tangent space to $\mathcal{M}$ at M is given by all matrices of the form $F_L^0\Delta_R^T + \Delta_L(F_R^0)^T$, where $\Delta_L, \Delta_R \in \mathbb{R}^{n\times(n-1)}$ are arbitrary. Therefore a matrix $H \in \mathbb{R}^{n\times n}$ is orthogonal to $\mathcal{M}$ at M if and only if $\langle F_L^0\Delta_R^T + \Delta_L(F_R^0)^T, H\rangle = \mathrm{tr}(\Delta_L(F_R^0)^T H^T + \Delta_R(F_L^0)^T H) = 0$ for all $\Delta_L, \Delta_R \in \mathbb{R}^{n\times(n-1)}$. Equivalently, $HF_R^0 = H^T F_L^0 = 0$, or $HM^T = H^T M = 0$. The assertion of the lemma now readily follows. □

Lemma 31. *Let $u^1, \dots, u^n \in \mathbb{R}^n$ be non-zero vectors, such that no two of these are proportional and the dimension of the linear span $\mathrm{span}\{u^1, \dots, u^n\}$ has corank at most 1. Then the rank 1 matrices $u^j(u^j)^T$, $j = 1, \dots, n$, are linearly independent.*

Proof. Without loss of generality we may assume that $u^1, \dots, u^{n-1}$ are linearly independent. In an appropriate coordinate system these vectors then equal the corresponding canonical basis vectors. Then $u^j(u^j)^T = E_{jj}$ for $j = 1, \dots, n-1$. Hence the rank 1 matrices $u^j(u^j)^T$ are linearly dependent only if $u^n(u^n)^T$ is diagonal with at least two non-zero entries, which leads to a contradiction. □

Lemma 32. *Define the set*

$$\mathcal{M} = \{S \in \mathcal{S}^n \mid \det S_{(1,\dots,n-1)} = \det S_{(2,\dots,n)} = \det(S_{ij})_{i=1,\dots,n-1;j=2,\dots,n} = 0\},$$

and let $S \in \mathcal{M}$ be a positive semi-definite matrix of corank 2. Suppose there exists a basis $\{u, v\} \subset \mathbb{R}^n$ of $\ker S$ such that $u_1 \neq 0$, $v_n \neq 0$, $u_n = v_1 = 0$. Then there exists a neighbourhood $\mathcal{U} \subset \mathcal{S}^n$ of S such that a matrix $S' \in \mathcal{U}$ is positive semi-definite of corank 2 if and only if $S' \in \mathcal{U} \cap \mathcal{M}$.

Proof. By $u_n = 0$ the subvector $u_{(1,\dots,n-1)}$ is in the kernel of $S_{(1,\dots,n-1)}$. Hence $S_{(1,\dots,n-1)}$ is of corank at least 1. If $w \in \ker S_{(1,\dots,n-1)}$ is another kernel vector, then $w' = (w^T, 0)^T \in \mathbb{R}^n$ is in the kernel of S and must therefore be proportional to u, because v cannot be in $\mathrm{span}\{u, w\}$ by $v_n \neq 0$. Therefore $S_{(1,\dots,n-1)}$ is positive semi-definite of corank 1. Similarly, the submatrix $S_{(2,\dots,n)}$ is positive semi-definite of corank 1.

Let $S' \in \mathcal{M}$ be close to S. Then by continuity the $n-2$ largest eigenvalues of $S'_{(1,\dots,n-1)}$ are positive, and the remaining eigenvalue is zero by definition of $\mathcal{M}$. Therefore $S'_{(1,\dots,n-1)} \succeq 0$ and $\mathrm{rk}\, S' \geq n-2$. The kernel of $S'_{(1,\dots,n-1)}$ is close to that of $S_{(1,\dots,n-1)}$, hence there exists a vector u', close to u, such that $(u')^T S' u' = 0$ and $u'_1 \neq 0$, $u'_n = 0$. Similarly, $S'_{(2,\dots,n)}$ is positive semi-definite and there exists a vector v', close to v, such that $(v')^T S' v' = 0$ and $v'_n \neq 0$, $v'_1 = 0$.

By $u'_1 \neq 0$ the first column of the submatrix $S'_{(1,\dots,n-1)}$ is a linear combination of the other columns. These $n-2$ columns must therefore be linearly independent. It follows that the submatrix $S'_{(2,\dots,n-1)}$ is positive definite. Therefore the $(n-2)\times(n-1)$ submatrix $(S'_{ij})_{i=2,\dots,n-1;j=2,\dots,n}$ has full row rank, and every vector in its right kernel must be proportional to $v'_{(2,\dots,n)}$. Hence the right kernel of the singular submatrix $(S'_{ij})_{i=1,\dots,n-1;j=2,\dots,n}$ must also be generated by $v'_{(2,\dots,n)}$. Similarly, the left kernel of this submatrix is generated by $u'_{(1,\dots,n-1)}$, and we get that $(u')^T S' v' = 0$.

By possibly replacing u' by $-u'$ or v' by $-v'$, we may enforce $u'_1 > 0$, $v'_n > 0$. By Lemma 29 we then have that S' is positive semi-definite. Now both u' and v' are in the kernel of S', and these vectors are linearly independent. Therefore $\mathrm{rk}\, S' \leq n-2$, and S' is of corank 2.

On the other hand, every matrix S' of corank 2 is in $\mathcal{M}$. This completes the proof. □

Lemma 33. *Let T be a singular real symmetric positive semi-definite Toeplitz matrix of rank k and with an element-wise nonnegative non-zero kernel vector u. Then there exist distinct angles $\zeta_0 = \pi$, $\zeta_1, \dots, \zeta_m \in (0, \pi)$ and positive numbers $\lambda_0, \dots, \lambda_m$, where $m = \lfloor \frac{k}{2} \rfloor$, such that $T = \sum_{j=0}^m \lambda_j T(\zeta_j)$ for odd k and $T = \sum_{j=1}^m \lambda_j T(\zeta_j)$ for even k, where $T(\zeta)$ is the symmetric Toeplitz matrix with first row $(1, \cos\zeta, \cos 2\zeta, \dots)$. Moreover, if $p(x)$ is the polynomial whose coefficients equal the entries of u, then $e^{\pm i\zeta_j}$ are roots of $p(x)$ for $j = 1, \dots, m$, and -1 is a root of $p(x)$ if k is odd.*

Proof. Any positive semi-definite Toeplitz matrix T of rank k can be represented as a weighted sum of k rank 1 positive semi-definite Toeplitz matrices with positive weights. Each of these rank 1 matrices is complex Hermitian with first row $(1, e^{i\zeta}, e^{2i\zeta}, \dots)$ for some $\zeta \in [0, 2\pi)$, and the angles ζ are pairwise distinct. If T is singular, then the weights and the angles are determined uniquely [21, Chapter 3]. For real T the complex rank 1 matrices appear in complex conjugate pairs, each of which sums to a Toeplitz matrix of the form $T(\zeta)$ with $\zeta \in (0, \pi)$.

The kernel of T equals the intersection of the kernels of the rank 1 summands. The angle $\zeta = 0$ then cannot appear in the sum due to the presence of an element-wise nonnegative non-zero kernel vector. Hence the angle $\zeta = \pi$, which corresponds to the only remaining real rank 1 Toeplitz matrix, appears in the sum if and only if k is odd.

Finally, u is in the kernel of every rank 1 summand in the decomposition of T. This directly yields the last assertion of the lemma. □

Lemma 34. *Assume the notations and conditions of the previous lemma and let $v \in \mathbb{R}^{k+1}$ be a non-zero kernel vector of the upper left principal submatrix of T of size $k+1$. Then v is proportional to the coefficient vector of the polynomial $p(x) = \prod_{j=1}^m (x^2 - 2x\cos\zeta_j + 1)$ if k is even and of the polynomial $p(x) = (x+1)\prod_{j=1}^m (x^2 - 2x\cos\zeta_j + 1)$ if k is odd.*

Proof. Let $v = (v_0, \dots, v_k)^T$. Since v is also in the kernel of the principal submatrix of each rank 1 component in the decomposition of T from the proof of the previous lemma, we have $\sum_{l=0}^k v_l e^{il\zeta_j} = 0$ for all $j = 0, \dots, m$ if k is odd, and for all $j = 1, \dots, m$ if k is even. This means that $e^{\pm i\zeta_j}$ are the roots of the polynomial $p_v(x) = \sum_{l=0}^k v_l x^l$ for all j. Since these are already k distinct roots, these must be all roots of p_v. Noting that $(x - e^{i\zeta})(x - e^{-i\zeta}) = x^2 - 2x\cos\zeta + 1$ and $x - e^{i\pi} = x + 1$ completes the proof. □

Lemma 35. *Let $n \geq 5, r, s$ be positive integers, $\gamma \in \mathbb{R}$ arbitrary, and $\zeta_1, \dots, \zeta_s \in [0, \pi]$. Then the system of r linear equations*

$$\begin{aligned} \sum_{j=1}^s \lambda_j (\cos(n-k)\zeta_j - \cos k\zeta_j) &= 0, \qquad k = \lceil \frac{n}{2} \rceil + 1 - r, \dots, \lceil \frac{n}{2} \rceil - 1, \\ \sum_{j=1}^s \lambda_j (\cos(n - (\lceil \frac{n}{2} \rceil - r))\zeta_j - \cos(\lceil \frac{n}{2} \rceil - r)\zeta_j) &= \gamma \end{aligned}$$

on the unknowns $\lambda_1, \dots, \lambda_s$ is equivalent to the system

$$\begin{pmatrix} 1 & \cdots & 1 \\ \cos\zeta_1 & \cdots & \cos\zeta_s \\ \vdots & & \vdots \\ \cos^{r-1}\zeta_1 & \cdots & \cos^{r-1}\zeta_s \end{pmatrix} \begin{pmatrix} \lambda_1 \sin\frac{\zeta_1}{2}\sin\frac{n\zeta_1}{2} \\ \vdots \\ \lambda_s \sin\frac{\zeta_s}{2}\sin\frac{n\zeta_s}{2} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -2^{-r}\gamma \end{pmatrix}$$

for odd n and

$$\begin{pmatrix} 1 & \cdots & 1 \\ \cos\zeta_1 & \cdots & \cos\zeta_s \\ \vdots & & \vdots \\ \cos^{r-1}\zeta_1 & \cdots & \cos^{r-1}\zeta_s \end{pmatrix} \begin{pmatrix} \lambda_1 \sin\zeta_1\sin\frac{n\zeta_1}{2} \\ \vdots \\ \lambda_s \sin\zeta_s\sin\frac{n\zeta_s}{2} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -2^{-r}\gamma \end{pmatrix}$$

for even n.

Proof. Due to the identity $\cos(2\alpha-\beta)-\cos\beta = -2\sin\alpha\sin(\alpha-\beta)$ the system is equivalent to

$$\begin{pmatrix} \sin(\frac{n}{2}-\lceil\frac{n}{2}\rceil+1)\zeta_1 & \cdots & \sin(\frac{n}{2}-\lceil\frac{n}{2}\rceil+1)\zeta_s \\ \vdots & & \vdots \\ \sin(\frac{n}{2}-\lceil\frac{n}{2}\rceil+r)\zeta_1 & \cdots & \sin(\frac{n}{2}-\lceil\frac{n}{2}\rceil+r)\zeta_s \end{pmatrix} \begin{pmatrix} \lambda_1\sin\frac{n\zeta_1}{2} \\ \vdots \\ \lambda_s\sin\frac{n\zeta_s}{2} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -\frac{\gamma}{2} \end{pmatrix}.$$

Column j of the coefficient matrix above is given by $(\sin\frac{\zeta_j}{2}, \sin\frac{3\zeta_j}{2}, \dots, \sin\frac{(2r-1)\zeta_j}{2})^T$ for odd n and by $(\sin\zeta_j, \sin 2\zeta_j, \dots, \sin r\zeta_j)^T$ for even n. Apply the formula $\sin k\varphi = \sin\varphi(e^{(k-1)i\varphi}+e^{(k-3)i\varphi}+\cdots+e^{-(k-1)i\varphi})$ to the coefficients in column j with $\varphi = \frac{\zeta_j}{2}$ for odd n and $\varphi=\zeta_j$ for even n.

By adding to each row of the coefficient matrix appropriate multiples of the rows above it, we may obtain a matrix whose column j is given by $\sin\frac{\zeta_j}{2}(1, e^{i\zeta_j}+e^{-i\zeta_j}, \dots, (e^{i\zeta_j}+e^{-i\zeta_j})^{r-1})^T$ for odd n and by $\sin\zeta_j(1, e^{i\zeta_j}+e^{-i\zeta_j}, \dots, (e^{i\zeta_j}+e^{-i\zeta_j})^{r-1})^T$ for even n. The right-hand side of the system does not change under this operation. Recalling that $e^{i\zeta}+e^{-i\zeta} = 2\cos\zeta$, we obtain the equivalent systems in the formulation of the lemma. □

Corollary 10. *Let $n \geq 5$ be an integer, and set $m = \lceil\frac{n}{2}\rceil - 2$. Let $\zeta_1, \dots, \zeta_m \in (0,\pi]$ be distinct angles. Then the inhomogeneous linear system of the m equations*

$$\begin{aligned} \sum_{j=1}^m \lambda_j(\cos(n-k)\zeta_j - \cos k\zeta_j) &= 0, \qquad 3 \leq k \leq m+1, \\ \sum_{j=1}^m \lambda_j(\cos(n-2)\zeta_j - \cos 2\zeta_j) &= -1 \end{aligned} \tag{26}$$

on the unknowns $\lambda_1, \dots, \lambda_m$ has a solution if and only if among the angles ζ_j there are no multiples of $\frac{2\pi}{n}$, and this solution is unique and given by

$$\lambda_j = \begin{cases} \left(2^m \sin\frac{\zeta_j}{2}\sin\frac{n\zeta_j}{2}\prod_{l\neq j}(\cos\zeta_j - \cos\zeta_l)\right)^{-1}, & n \text{ odd}, \\ \left(2^m \sin\zeta_j\sin\frac{n\zeta_j}{2}\prod_{l\neq j}(\cos\zeta_j - \cos\zeta_l)\right)^{-1}, & n \text{ even}. \end{cases} \tag{27}$$

Proof. Apply Lemma 35 with $r = s = m$. Since the cosine function is strictly monotonous on $(0, \pi]$, the Vandermonde matrix in the equations in this lemma is non-singular. Using explicit formulas for the inverse of the Vandermonde matrix [18], we obtain for every $j = 1, \dots, m$ that $\lambda_j \sin \frac{\zeta_j}{2} \sin \frac{n\zeta_j}{2} = \frac{1}{2^m \prod_{l \neq j}(\cos \zeta_j - \cos \zeta_l)}$ for odd n and $\lambda_j \sin \zeta_j \sin \frac{n\zeta_j}{2} = \frac{1}{2^m \prod_{l \neq j}(\cos \zeta_j - \cos \zeta_l)}$ for even n. The claim of the corollary now easily follows. □

B Extremality of exceptional circulant matrices

In this section we provide Lemma 38, which is the technically most difficult part of the proof of Lemma 26. Its proof uses a bit more advanced mathematical concepts, in particular, linear group representations.

Let $L_C \subset \mathcal{S}^n$ be the subspace of circulant matrices, i.e., matrices which are invariant with respect to simultaneous circular shifts of the row and column indices. Let $P_S : \mathcal{S}^n \to \mathcal{S}^n$ be the linear map which corresponds to a circular shift by one entry. Then P_S^n is the identity map Id, and P_S generates a symmetry group which is isomorphic to the cyclic group C_n. However, symmetric circulant matrices possess yet another symmetry. Namely, they are *persymmetric*, i.e., invariant with respect to reflection about the main skew diagonal. Denote this reflection by $P_P : \mathcal{S}^n \to \mathcal{S}^n$. The symmetry group generated by P_S and P_P is isomorphic to the dihedral group D_n, which has $2n$ elements. The action of D_n on $\mathcal{S}^n$ defines a linear unitary representation $R_{\mathcal{S}^n}$ of D_n of dimension $\frac{n(n+1)}{2}$, which decomposes into a direct sum of irreducible representations. This decomposition corresponds to an orthogonal decomposition of $\mathcal{S}^n$ into a direct sum of invariant subspaces.

In this section we suppose $n \geq 5$ to be an odd number. Then the group D_n has two irreducible representations of dimension 1. Both of these send P_S to the identity Id. The element P_P is sent to Id by the trivial representation and to $-Id$ by the other 1-dimensional representation. The $\frac{n+1}{2}$-dimensional subspace L_C is exactly the invariant subspace corresponding to the trivial representation. The other 1-dimensional representation does not participate in $R_{\mathcal{S}^n}$, because there is no non-zero matrix $A \in \mathcal{S}^n$ such that $P_S(A) = A$ and $P_P(A) = -A$. Besides the 1-dimensional representations, D_n possesses $\frac{n-1}{2}$ 2-dimensional representations $R_1, \dots, R_{\frac{n-1}{2}}$. Here R_k sends P_S to the rotation of the 2-dimensional representing subspace by the angle $\frac{2\pi k}{n}$, and P_P to a reflection of this subspace.

Set $m = \frac{n-3}{2}$ and let $\zeta_1, \dots, \zeta_m \in (0, \pi)$ be distinct angles in increasing order. Define the polynomial $p(x) = \prod_{j=1}^m (x^2 - 2x \cos \zeta_j + 1)$, which has roots $e^{\pm i\zeta_j}$, and let $u \in \mathbb{R}^{n-2}$ be its coefficient vector. Note that p is palindromic, i.e., u does not change if the order of its entries in inverted. For $j = 1, \dots, n$, define vectors $u^j \in \mathbb{R}^n$ such that $u^j_{I_j} = u$ and $u^j_i = 0$ for all $i \notin I_j$. We do not make further assumptions on the collection $\mathbf{u} = \{u^1, \dots, u^n\}$, in particular, we do not demand u to be positive.

For every $k = 1, \dots, \frac{n-1}{2}$ we also define the polynomial $p_k(x) = \prod_{j=1}^m (x^2 - 2xe^{-\pi ik(n-1)/n} \cos \zeta_j + e^{-2\pi ik(n-1)/n})$ and denote by $v^k \in \mathbb{R}^{n-2}$ its coefficient vector, with $v^k_1 = 1$ being the coefficient at x^{2m}. Then the roots of p_k all lie on the unit circle and equal $e^{i(\pm\zeta_j - \pi k(n-1)/n)}$, $j = 1, \dots, m$, and the elements of v^k are given by $v^k_l = e^{\pi ik(n+1-l)(n-1)/n} u_l$, $l = 1, \dots, n-2$.

For given $\mathbf{u}$, defined by angles $\zeta_1, \dots, \zeta_m$ as above, we are interested in the linear subspace $L_{\mathbf{u}} \subset \mathcal{S}^n$ of symmetric matrices A such that $A_{I_j} u = 0$ for all $j = 1, \dots, n$. If $A \in L_{\mathbf{u}}$ is a solution of the corresponding linear system of equations, then the matrices $P_S^k(A)$ obtained from A by circular shifts of the row and column indices are also solutions. Moreover, since u is palindromic, $P_P(A)$ is a solution too. Therefore $L_{\mathbf{u}}$ is an invariant subspace under the action of the group D_n, and this action defines a linear representation $R_{\mathbf{u}}$ of D_n on $L_{\mathbf{u}}$. This representation decomposes into a direct sum of irreducible representations and induces an orthogonal decomposition of $L_{\mathbf{u}}$ into a direct sum of invariant subspaces $L_{\mathbf{u},Id}, L_{\mathbf{u},k}$, $k = 1, \dots, \frac{n-1}{2}$, corresponding to the trivial irreducible representation and the representations R_k of D_n. As noticed above, the non-trivial 1-dimensional representation of D_n does not contribute to $R_{\mathcal{S}^n}$ and hence neither to $R_{\mathbf{u}}$.

The subspace $L_{\mathbf{u},Id}$ then consists exactly of those matrices A which are circulant and satisfy $A_{I_1}u = 0$. The next result characterizes the subspaces $L_{\mathbf{u},k}$.

Lemma 36. *Let $A \in L_{\mathbf{u},k}$ be a non-zero matrix. Then there exists a complex symmetric matrix B such that $ReB, ImB \in L_{\mathbf{u},k}$, $A \in \operatorname{span}\{ReB, ImB\}$, and B can be represented as a Hadamard product $B = C \circ H$ of a non-zero real symmetric circulant matrix C and a Hankel rank 1 matrix H given element-wise by $H_{jl} = e^{\pi ik(n+1-j-l)(n-1)/n}$. Moreover, we have $C_{I_1}v^k = 0$.*

Proof. Let L be a 2-dimensional subspace which is invariant under the action of D_n and such that $A \in L \subset L_{\mathbf{u},k}$. Then the action of D_n on L is given by the representation R_k, i.e., there exists a basis $\{B_1, B_2\}$ of L such that

$$\begin{pmatrix} P_S(B_1) \\ P_S(B_2) \end{pmatrix} = \begin{pmatrix} \cos\frac{2\pi k}{n} & \sin\frac{2\pi k}{n} \\ -\sin\frac{2\pi k}{n} & \cos\frac{2\pi k}{n} \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}, \qquad \begin{pmatrix} P_P(B_1) \\ P_P(B_2) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}.$$

Setting $B = B_1 + iB_2$, we obtain that $P_S(B) = e^{-2\pi ik/n}B$, $P_P(B) = \overline{B}$.

The first condition is equivalent to the condition $B_{jl} = e^{2\pi ik/n}B_{j_-l_-}$ for all $j, l = 1, \dots, n$, where $j_-, l_- \in \{1, \dots, n\}$ are the unique indices satisfying $j_- \equiv j - 1$ and $l_- \equiv l - 1$ modulo n. For every $j, l = 1, \dots, n$ we then have

$$B_{jl} = \begin{cases} \exp\left(\frac{2\pi ik}{n}\frac{j+l-n-1}{2}\right) \cdot B_{j-\frac{j+l-n-1}{2},l-\frac{j+l-n-1}{2}}, & (j+l) \text{ even}; \\ \exp\left(\frac{2\pi ik}{n}\frac{j+l-1}{2}\right) \cdot B_{j+n-\frac{j+l-1}{2},l-\frac{j+l-1}{2}}, & j < l,\ (j+l) \text{ odd}; \\ \exp\left(\frac{2\pi ik}{n}\frac{j+l-1}{2}\right) \cdot B_{j-\frac{j+l-1}{2},l+n-\frac{j+l-1}{2}}, & j > l,\ (j+l) \text{ odd}. \end{cases}$$

Since n is odd, the first factors in this representation of the elements of B form the Hankel matrix H, while the second factors form a circulant matrix C which coincides with B on the main skew-diagonal. However, the condition $P_P(B) = \overline{B}$ implies that the elements on the main skew diagonal of B are real. Hence C is also real. This yields the claimed representation $B = C \circ H$. Since $B \neq 0$, we also have $C \neq 0$.

Since $B_1, B_2 \in L_{\mathbf{u}}$, we have that $B_{I_1}u = 0$. However, for all $l = 1, \dots, n-2$ we have $(B_{I_1}u)_l = e^{-\pi ikl(n-1)/n}(C_{I_1}v^k)_l$ by definition of v^k, and hence also $C_{I_1}v^k = 0$. This completes the proof. □

Recall that for a circulant matrix A, the submatrix A_{I_1} is Toeplitz. The next result shows that the conditions $Tu = 0$ or $Tv^k = 0$ impose stringent constraints on a real symmetric Toeplitz matrix T.

Lemma 37. *Let $\varphi_1, \dots, \varphi_d \in (-\pi, \pi]$ be distinct angles, and let $w \in \mathbb{R}^{d+1}$ be the coefficient vector of the polynomial $p(x) = \prod_{k=1}^{d}(x - e^{i\varphi_k})$, with $w_1 = 1$ being the coefficient at x^d. Let $\Xi \subset [0, \pi]$ be the set of angles ξ such that either both $\pm\xi$ appear among the angles φ_k, $k = 1, \dots, d$, or $\xi = \varphi_j = \pi$ for some j. Let T be a real symmetric Toeplitz matrix satisfying $Tw = 0$. Then $T \in \operatorname{span}\{T_\xi\}_{\xi\in\Xi}$, where T_ξ is the symmetric Toeplitz matrix with first row $(1, \cos\xi, \dots, \cos d\xi)$.*

Proof. Let $\varphi_{d+1}, \dots, \varphi_{2d+1} \in (-\pi, \pi]$ be such that φ_j are mutually distinct for $j = 1, \dots, 2d+1$. For any $\varphi \in (-\pi, \pi]$, let $h_\varphi = (e^{ik\varphi})_{k=0,\dots,d} \in \mathbb{C}^{d+1}$ be a column vector and $H_\varphi = h_\varphi h_\varphi^*$ the corresponding complex Hermitian rank 1 Toeplitz matrix. Then $H_{\varphi_1}, \dots, H_{\varphi_{2d+1}}$ are linearly independent over the complex numbers, and hence also over the reals. Indeed, the matrix H_φ contains $2d+1$ distinct elements $e^{-id\varphi}, \dots, e^{id\varphi}$. However, the vectors $(e^{-id\varphi_j}, \dots, e^{id\varphi_j})$, $j = 1, \dots, 2d+1$, are linearly independent, because suitable multiples of these vectors can be arranged into a Vandermonde matrix. Therefore $H_{\varphi_1}, \dots, H_{\varphi_{2d+1}}$ form a basis of the $(2d+1)$-dimensional real vector space of complex Hermitian $(d+1) \times (d+1)$ Toeplitz matrices.

The real symmetric Toeplitz matrix T is also complex Hermitian and can hence be written as a linear combination $T = \sum_{j=1}^{2d+1} \alpha_j H_{\varphi_j}$, $\alpha_j \in \mathbb{R}$. Now $h_{\varphi_j}^* w = 0$ for $j = 1, \dots, d$ by construction of w, and therefore $Tw = \sum_{j=d+1}^{2d+1} \alpha_j (h_{\varphi_j}^* w) h_{\varphi_j} = 0$. But the vectors $h_{\varphi_{d+1}}, \dots, h_{\varphi_{2d+1}}$ again form a Vandermonde matrix and are hence linearly independent. Moreover, we have $h_{\varphi_j}^* w = e^{-id\varphi_j} p(e^{i\varphi_j}) \neq 0$ for all $j = d+1, \dots, 2d+1$. It follows that $\alpha_j = 0$ for all $j = d+1, \dots, 2d+1$, and $T = \sum_{j=1}^{d} \alpha_j H_{\varphi_j}$.

Now the first column of the imaginary part $Im H_{\varphi_j}$ is given by $Im h_{\varphi_j} = (0, \sin\varphi_j, \dots, \sin d\varphi_j)^T$, and hence $\sum_{j=1}^{d} \alpha_j \sin l\varphi_j = 0$ for all $l = 1, \dots, d$. As in the proof of Lemma 35, we may use the formula $\sin l\varphi = \sin\varphi(e^{(l-1)i\varphi} + e^{(l-3)i\varphi} + \dots + e^{-(l-1)i\varphi})$ to rewrite this system of linear equations on the coefficients α_j as

$$\begin{pmatrix} 1 & \cdots & 1 \\ \cos\varphi_1 & \cdots & \cos\varphi_d \\ \vdots & & \vdots \\ \cos^{d-1}\varphi_1 & \cdots & \cos^{d-1}\varphi_d \end{pmatrix} \begin{pmatrix} \alpha_1 \sin\varphi_1 \\ \vdots \\ \alpha_d \sin\varphi_d \end{pmatrix} = 0.$$

It follows that a coefficient α_j can only be non-zero if either $\sin\varphi_j = 0$, in which case $\varphi_j \in \Xi$ and $H_{\varphi_j} = T_{\varphi_j}$, or there exists another index $j' \in \{1, \dots, d\}$ such that $\varphi_{j'} = -\varphi_j$ and $\alpha_{j'} = \alpha_j$, and therefore $|\varphi_j| \in \Xi$ and $\alpha_j H_{\varphi_j} + \alpha_{j'} H_{\varphi_{j'}} = 2\alpha_j T_{|\varphi_j|}$. This completes the proof. $\square$

The restrictions on the Toeplitz matrices translate into the following restrictions on matrices $A \in L_{\mathbf{u},Id}$ and on the circulant factor in Lemma 36.

Corollary 11. *Let $n \geq 5$ be an odd integer, set $m = \frac{n-3}{2}$, and let $\varphi_1, \dots, \varphi_{2m} \in (-\pi, \pi]$ be distinct angles, such that there are no multiples of $\frac{2\pi}{n}$ among them. Define the vector $w \in \mathbb{R}^{n-2}$ and the set $\Xi \subset [0, \pi]$ as in Lemma 37, with $d = 2m$.*

Let $L_w \subset L_C$ be the linear subspace of real symmetric circulant matrices C such that $C_{I_1} w = 0$. Then $\dim L_w \leq 1$. If $\dim L_w = 1$, then Ξ has m elements. In particular, for $\dim L_w = 1$ either the values $e^{i\varphi_j}$ group into m complex-conjugate pairs, or they group into $m-1$ complex conjugate pairs and among the two remaining values one equals -1.

Proof. Since $\varphi_j \neq 0$ for all $j = 1, \dots, 2m$, the set Ξ can have at most m elements. Set $r = |\Xi|$.

Let $C \in L_w$ be non-zero. By Lemma 37 the Toeplitz matrix $T = C_{I_1}$ can be written as a non-zero linear combination of $\{T_\xi\}_{\xi \in \Xi}$, $T = \sum_{j=1}^{r} \lambda_j T_{\xi_j}$, $\xi_j \in \Xi$ for all $j = 1, \dots, r$. Since the elements of C_{I_1} determine the circulant matrix C completely by Lemma 3, we also have $\dim L_w \leq r$. Since $C \neq 0$, the set Ξ contains at least one element.

For $n = 5$ we then get $r = m = 1$, which proves the assertion in this case.

Suppose that $n \geq 7$. We have $C_{1k} = C_{1,n+2-k}$ for all $k = 2, \dots, n$. It follows that $T_{1k} = T_{1,n+2-k}$ for all $k = 4, \dots, \frac{n+1}{2}$. This yields the linear homogeneous system of equations $\sum_{j=1}^{r} \lambda_j \cos k\xi_j =$

$\sum_{j=1}^{r} \lambda_j \cos(n-k)\xi_j$, $k = 3, \dots, \frac{n-1}{2}$, on the coefficients λ_j. By Lemma 35 this system is equivalent to the system

$$\begin{pmatrix} 1 & \cdots & 1 \\ \cos\xi_1 & \cdots & \cos\xi_r \\ \vdots & & \vdots \\ \cos^{m-2}\xi_1 & \cdots & \cos^{m-2}\xi_r \end{pmatrix} \begin{pmatrix} \lambda_1 \sin\frac{\xi_1}{2}\sin\frac{n\xi_1}{2} \\ \vdots \\ \lambda_r \sin\frac{\xi_r}{2}\sin\frac{n\xi_r}{2} \end{pmatrix} = 0.$$

Since there are no multiples of $\frac{2\pi}{n}$ among the angles φ_j, there are no multiples of $\frac{2\pi}{n}$ among the ξ_j neither, and hence $\sin\frac{\xi_j}{2}\sin\frac{n\xi_j}{2} \neq 0$ for all $j = 1, \dots, r$. It follows that the coefficient matrix in the system above has a non-trivial kernel, implying $r > m-1$ and hence $r = m$.

However, the coefficient matrix has full row rank $m-1$, and therefore the solution $\lambda_1, \dots, \lambda_m$ is determined by the angles $\xi_1, \dots, \xi_m$ up to multiplication by a common scalar. Hence C_{I_1} and by Lemma 3 also C is determined up to a scalar factor, and $\dim L_w \leq 1$. □

We are now in a position to prove the result we need for Lemma 26.

Lemma 38. *Let $n \geq 5$ be odd. Set $m = \frac{n-3}{2}$ and let $\zeta_1, \dots, \zeta_m \in (0, \pi)$ be distinct angles in increasing order such that the fractional part of $\frac{n\zeta_j}{4\pi}$ is in $(0, \frac{1}{2})$ for odd j and in $(\frac{1}{2}, 1)$ for even j. Let $u \in \mathbb{R}^{n-2}$ be the coefficient vector of the polynomial $p(x) = \prod_{j=1}^{m}(x^2 - 2x\cos\zeta_j + 1)$ and let $L_{\mathbf{u}} \subset \mathcal{S}^n$ be the subspace of all matrices A satisfying $A_{I_j}u = 0$ for all $j = 1, \dots, n$. Then the condition $\dim L_{\mathbf{u}} > 1$ implies that $\zeta_j = \frac{(2j-1)\pi}{n}$ for all $j = 1, \dots, m$. In particular, the vector u has negative elements.*

Proof. By assumption there are no multiples of $\frac{2\pi}{n}$ among the angles $\pm\zeta_j$ and, since $n-1$ is even, also among the angles $\pm\zeta_j - \frac{\pi k(n-1)}{n}$ for all $j = 1, \dots, m$ and $k = 1, \dots, \frac{n-1}{2}$. Note also that $\frac{\pi k(n-1)}{n}$ is not a multiple of 2π for these values of k, and hence the angles $\pm\zeta_j - \frac{\pi k(n-1)}{n}$ are obtained from the angles $\pm\zeta_j$ by a shift by a non-zero value modulo 2π.

The solution space $L_{\mathbf{u}}$ is a direct sum of the subspaces $L_{\mathbf{u},Id}$ and $L_{\mathbf{u},k}$, $k = 1, \dots, \frac{n-1}{2}$ corresponding to the irreducible representations of the group D_n. By Corollary 11 with $w = u$ we have $\dim L_{\mathbf{u},Id} \leq 1$. Therefore $\dim L_{\mathbf{u}} > 1$ implies that $L_{\mathbf{u},k}$ is non-zero for some k.

Let $A \in L_{\mathbf{u},k}$ be a non-zero matrix. Then by Lemma 36 there exists a non-zero real symmetric circulant matrix C satisfying $C_{I_1}v^k = 0$. By Corollary 11 with $w = v^k$ the roots $e^{i(\pm\zeta_j - \pi k(n-1)/n)}$, $j = 1, \dots, m$, of $p_k(x)$ either group into m complex-conjugate pairs, or they group into $m-1$ complex conjugate pairs and among the two remaining roots one equals -1. We shall now show that this condition uniquely determines the angles ζ_j.

For $l = 1, \dots, n$, define open arcs $a_l = \{e^{i\varphi} \mid \varphi \in (\frac{2\pi(l-1)}{n}, \frac{2\pi l}{n})\}$ of length $\frac{2\pi}{n}$ on the unit circle. Then $e^{\pm i\zeta_j}, e^{i(\pm\zeta_j - \pi k(n-1)/n)} \in \bigcup_{l=1}^{n} a_l$ for all $j = 1, \dots, m$, $k = 1, \dots, \frac{n-1}{2}$. Moreover, by the assumptions on ζ_j we can have $e^{i\zeta_j} \in a_l$ only if the parity condition $l \equiv j$ modulo 2 holds. Since $\zeta_1, \dots, \zeta_m$ is an increasing sequence, we also have that each interval a_l contains at most one of the values $e^{i\zeta_1}, \dots, e^{i\zeta_m}$. We consider two cases.

1. $\zeta_m > \frac{(n-1)\pi}{n}$. Then $e^{\pm i\zeta_m} \in a_{(n+1)/2}$. Any other arc a_l contains at most one of the values $e^{\pm i\zeta_j}$. Hence there are exactly 4 of these arcs containing no such value, and these are located symmetrically about the real axis. Now consider how the rotated values $e^{i(\pm\zeta_j - \pi k(n-1)/n)}$, $j = 1, \dots, m$, are distributed over the arcs a_l. In a similar way there must be 4 arcs, call them $\alpha_1, \alpha_2, \alpha_3, \alpha_4$, containing

no value and one arc, call it β, containing two values, but $\beta \neq a_{(n+1)/2}$. We distinguish again two possibilities.

1.1. If the complex conjugate arc to β is one of the arcs $\alpha_1, \dots, \alpha_4$, then the two complex values contained in β are not matched by complex conjugate values.

1.2. If none of the arcs $\alpha_1, \dots, \alpha_4$ is complex conjugate to β, then at least one of these arcs, let it be α_1, is matched by a complex conjugate arc containing exactly one value. Hence at least one of the values in β and the value in the complex conjugate arc to α_1 are not matched by complex conjugate values.

It follows in both cases that there are at least two complex values among $e^{i(\pm\zeta_j - \pi k(n-1)/n)}$ which are not matched by a complex conjugate, leading to a contradiction.

2. $\zeta_m < \frac{(n-1)\pi}{n}$. Since $e^{i\zeta_m} \notin a_{m+1}$ by the parity condition, we must have $e^{i\zeta_j} \in a_j$, $e^{-i\zeta_j} \in a_{n+1-j}$ for all $j = 1, \dots, m$. Consider again the distribution of the values $e^{i(\pm\zeta_j - \pi k(n-1)/n)}$, $j = 1, \dots, m$. There are 3 consecutively located arcs which do not contain any of the values $e^{i(\pm\zeta_j - \pi k(n-1)/n)}$, call them $\alpha_1, \alpha_2, \alpha_3$. The remaining arcs contain exactly one value each. The arcs $\alpha_1, \alpha_2, \alpha_3$ are obtained from the arcs $a_{(n-1)/2}, a_{(n+1)/2}, a_{(n+3)/2}$ by multiplication with $e^{-i\pi k(n-1)/n}$ and are not located symmetrically about the real axis. Hence at least one value among $e^{i(\pm\zeta_j - \pi k(n-1)/n)}$, $j = 1, \dots, m$, is not matched by a complex conjugate. It follows that among these values the value -1 must appear, and two of the arcs $\alpha_1, \alpha_2, \alpha_3$ must be complex conjugate to each other. The second condition is only possible if these two arcs border the point $z = 1$ on the unit circle. Equivalently, $e^{i\pi k(n-1)/n}$ must lie on the boundary of the arc $a_{(n+1)/2}$, implying $k = 1$. Recall that the value among $e^{i(\pm\zeta_j - \pi(n-1)/n)}$, $j = 1, \dots, m$ which lies in the interval $a_{(n+1)/2}$ must equal -1. This is the value $e^{i(-\zeta_1 - \pi(n-1)/n)}$, and hence $\zeta_1 = \frac{\pi}{n}$. Finally, using that the values $e^{i(\zeta_j - \pi(n-1)/n)}$ and $e^{i(-\zeta_{j+1} - \pi(n-1)/n)}$ are mutually complex conjugate for all $j = 1, \dots, m-1$, we obtain the values $\zeta_j = \frac{(2j-1)\pi}{n}$ for all $j = 1, \dots, m$.

Thus we have $p(x) = \prod_{j=1}^m (x^2 - 2x\cos\frac{(2j-1)\pi}{n} + 1)$. The coefficient at the linear term is given by $u_1 = -2\sum_{j=1}^m \cos\frac{(2j-1)\pi}{n} < 0$, which concludes the proof. □

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