



## EXTREMAL COPOSITIVE MATRICES WITH ZERO SUPPORTS OF CARDINALITY $N - 2^*$

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**Abstract.** Let  $A \in \mathcal{C}^n$  be an exceptional extremal copositive  $n \times n$  matrix with positive diagonal. A zero  $u$  of  $A$  is a non-zero nonnegative vector such that  $u^T A u = 0$ . The support of a zero  $u$  is the index set of the positive elements of  $u$ . A zero  $u$  is minimal if there is no other zero  $v$  such that  $\text{supp } v \subset \text{supp } u$  strictly. Let  $G$  be the graph on  $n$  vertices which has an edge  $(i, j)$  if and only if  $A$  has a zero with support  $\{1, \dots, n\} \setminus \{i, j\}$ . In this paper, it is shown that  $G$  cannot contain a cycle of length strictly smaller than  $n$ . As a consequence, if all minimal zeros of  $A$  have support of cardinality  $n - 2$ , then  $G$  must be the cycle graph  $C_n$ .

**Key words.** Copositive matrix, Extreme ray, Zero support set.

**AMS subject classifications.** 15A48, 15A21.

**1. Introduction.** An element  $A$  of the space  $\mathcal{S}^n$  of real symmetric  $n \times n$  matrices is called *copositive* if  $x^T A x \geq 0$  for all vectors  $x \in \mathbb{R}_+^n$ . The set of such matrices forms the *copositive cone*  $\mathcal{C}^n$ . This cone plays an important role in non-convex optimization, as many difficult optimization problems can be reformulated as conic programs over  $\mathcal{C}^n$ . For a detailed survey of the applications of this cone see, e.g., [3, 9].

Verifying copositivity of a given matrix is a co-NP-complete problem [12], and the complexity of the copositive cone quickly grows with dimension. In this note, we focus on the extreme rays of  $\mathcal{C}^n$ . A non-zero matrix  $A \in \mathcal{C}^n$  is called *extremal* if a decomposition  $A = A_1 + A_2$  of  $A$  into matrices  $A_1, A_2 \in \mathcal{C}^n$  is only possible if  $A_1 = \lambda A$ ,  $A_2 = (1 - \lambda)A$  for some  $\lambda \in [0, 1]$ . The extremal matrix is called *exceptional* if it is neither element-wise nonnegative nor positive semi-definite. The set of positive multiples of an extremal matrix is called an *extreme ray* of  $\mathcal{C}^n$ . The set of extreme rays is an important characteristic of a convex cone. Its structure, first of all its stratification into a union of manifolds of different dimension, yields much information about the shape of the cone. The extreme rays of a convex cone which is algorithmically difficult to access are especially important if one wishes to check the tightness of inner convex approximations of the cone. Namely, an inner approximation is exact if and only if it contains all extreme rays. Since the extreme rays of a cone determine the facets of its dual cone, they are also important tools for the study of this dual cone. The extreme rays of the copositive cone have been used in a number of papers on its dual, the completely positive cone [4, 5, 7, 13, 14, 15].

A useful tool in the study of extremal copositive matrices are its zeros [2, 6]. A *zero*  $u$  of a copositive matrix  $A$  is a non-zero nonnegative vector such that  $u^T A u = 0$ . The *support*  $\text{supp } u$  of a zero  $u = (u_1, \dots, u_n)^T \in \mathbb{R}_+^n$  is the subset of indices  $j \in \{1, \dots, n\}$  such that  $u_j > 0$ . The *zero support set*, i.e., the ensemble of zero supports of a copositive matrix is an informative characteristic of the matrix. In particular, this combinatorial characteristic can assist the classification of the extreme rays of  $\mathcal{C}^n$ . A zero  $u$  of  $A$  is called *minimal* if there is no zero  $v$  of  $A$  such that  $\text{supp } v \subset \text{supp } u$  holds strictly.

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By [8, Corollary 4.14], an exceptional extremal copositive matrix in  $\mathcal{C}^n$  cannot have zero supports with cardinality  $\geq n - 1$ . In this note we constrain the zero support set of exceptional extremal copositive matrices with positive diagonal, in particular the subset of supports of cardinality  $n - 2$ . This subset can be conveniently represented by a graph  $G$  on  $n$  vertices, a support  $\{1, \dots, n\} \setminus \{i, j\}$  defining an edge  $(i, j)$  of  $G$ . We show that the graph  $G$  cannot contain cycles of length strictly smaller than  $n$ . This allows us to completely describe the graph  $G$  for extremal copositive  $n \times n$  matrices whose minimal zero supports have all cardinality  $n - 2$ . Namely, in this case, the graph has to be the cycle graph  $C_n$ , and the study of the corresponding extremal exceptional copositive matrices is reduced to the case treated in the paper [11].

**2. Notations and preliminaries.** We shall denote vectors with lower-case letters and matrices with upper-case letters. Individual entries of a vector  $u$  or a matrix  $A$  will be denoted by  $u_i$ ,  $A_{ij}$ , respectively. For a matrix  $A$  and a vector  $u$  of compatible size, the  $i$ -th element of the vector  $Au$  will be denoted by  $(Au)_i$ . Inequalities  $u \geq 0$  on vectors will be meant element-wise, the inequality  $A \succeq 0$  means that  $A$  is positive semi-definite. The cone of positive semi-definite real symmetric  $n \times n$  matrices will be denoted by  $\mathcal{S}_+^n$ .

For a subset  $I \subset \{1, \dots, n\}$ , we denote by  $A_I$  the principal submatrix of  $A$  whose elements have row and column indices in  $I$ , i.e.,  $A_I = (A_{ij})_{i,j \in I}$ . Similarly for a vector  $u \in \mathbb{R}^n$  we define the subvector  $u_I = (u_i)_{i \in I}$ . The index set  $\{1, \dots, n\} \setminus I$  will be denoted by  $\bar{I}$ .

Let  $A \in \mathcal{C}^n$ , and define the graph  $G$  on  $n$  vertices as follows. There exists an edge  $(i, j)$  in  $G$  if and only if  $\{1, \dots, n\} \setminus \{i, j\}$  is the support of some zero of  $A$ . A *cycle* of length  $k$  in  $G$  is a subset of  $k \geq 3$  edges  $(i_1, i_2), (i_2, i_3), \dots, (i_{k-1}, i_k), (i_k, i_1)$ , where the  $i_1, \dots, i_k \in \{1, \dots, n\}$  are mutually distinct vertices.

We shall consider exceptional extremal matrices  $A \in \mathcal{C}^n$  such that the graph  $G$  has a cycle of length  $k$ ,  $3 \leq k \leq n - 1$ . Without loss of generality we may assume that  $i_j = j$ ,  $j = 1, \dots, k$ . Define the index subsets  $I_0 = \{k + 1, \dots, n\}$ ,  $I_j = \{1, \dots, n\} \setminus \{j, j + 1\}$ ,  $j = 1, \dots, k - 1$ , and  $I_k = \{1, \dots, n\} \setminus \{k, 1\}$ . Then  $I_1, \dots, I_k$  are zero supports of  $A$  and  $I_0$  is their intersection. Let  $u^1, \dots, u^k$  be zeros of  $A$  with supports  $I_1, \dots, I_k$ , respectively. Define also the index subsets  $I'_j = I_j \setminus I_0 \subset \{1, \dots, k\}$ ,  $j = 1, \dots, k$ .

Let further  $\mathcal{N}^n \subset \mathcal{S}^n$  be the cone of element-wise nonnegative real symmetric  $n \times n$  matrices.

We now collect some results from the literature that will be used later on.

LEMMA 2.1. [8, Lemma 2.4] *Let  $A \in \mathcal{C}^n$  and let  $u$  be a zero of  $A$ . Then the principal submatrix  $A_{\text{supp } u}$  is positive semi-definite.*

LEMMA 2.2. [8, Lemma 2.5] *Let  $A \in \mathcal{C}^n$  and let  $u$  be a zero of  $A$ . Then  $(Au)_i = 0$  for all  $i \in \text{supp}(u)$ .*

LEMMA 2.3. [2, p. 200] *Let  $A \in \mathcal{C}^n$  and let  $u$  be a zero of  $A$ . Then  $Au \geq 0$ .*

The following result is a consequence of [8, Corollary 4.14].

LEMMA 2.4. *An exceptional extremal copositive matrix in  $\mathcal{C}^n$  cannot have zero supports with cardinality  $\geq n - 1$ .*

The following result is a consequence of [11, Theorem 2.9].

THEOREM 2.5. *Assume above notations. Let  $k \geq 5$  and let  $B \in \mathcal{S}^k$  be such that for every  $j = 1, \dots, k$  there exists a nonnegative vector  $v^j$  with  $\text{supp } v^j = I'_j$  satisfying  $(v^j)^T B v^j = 0$ . Then the following are equivalent:*

- (i)  $B$  is copositive;

(ii)  $B_{I_j'}$  is positive semi-definite for  $j = 1, \dots, k$ ,  $(v^k)^T B v^1 \geq 0$ , and  $(v^j)^T B v^{j+1} \geq 0$  for  $j = 1, \dots, k-1$ .

The following result is a consequence of [10, Lemma 3.5].

LEMMA 2.6. *Let  $A$  be a copositive matrix and  $u, v$  minimal zeros of  $A$  such that  $\text{supp } u = \text{supp } v$ . Then  $u, v$  are proportional.*

LEMMA 2.7. [10, Corollary 3.12] *Let  $A$  be a copositive matrix and  $u, v$  minimal zeros of  $A$  with supports  $\text{supp } u = I$ ,  $\text{supp } v = J$ . Assume that  $J \setminus I = \{k\}$  consists of one element. Then every zero  $w$  of  $A$  with support  $\text{supp } w \subset I \cup J$  can be represented as a convex conic combination  $w = \alpha u + \beta v$  with  $\alpha, \beta \geq 0$ . In particular, up to multiplication by a positive constant, there are no minimal zeros  $w$  with  $\text{supp } w \subset I \cup J$  other than  $u$  and  $v$ .*

The following result is a consequence of [10, Theorem 4.5].

LEMMA 2.8. *Let  $A \in \mathcal{C}^n$  be exceptional extremal. Then the number of linearly independent minimal zeros of  $A$  has to be at least  $n$ .*

We shall now introduce the generalized Schur complement. For more information see [1].

Let  $A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \in \mathcal{S}^{n_1+n_2}$  be a real symmetric matrix partitioned into 4 blocks. Suppose that  $A_{22}$  is positive semi-definite, and  $\ker A_{22} \subset \ker A_{12}$ . Let  $r$  be the rank of  $A_{22}$ , and let  $F_2 \in \mathbb{R}^{r \times n_2}$  be a factor such that  $A_{22} = F_2^T F_2$ . Since the row space of  $A_{12}$  is contained in the row space of  $A_{22}$  and the latter equals the row space of  $F_2$ , we find a  $r \times n_1$  matrix  $F_1$  such that  $A_{12} = F_1^T F_2$ .

DEFINITION 2.9. Assume above conditions and notations. The difference  $B = A_{11} - F_1^T F_1 \in \mathcal{S}^{n_1}$  is called the *generalized Schur complement* of  $A_{22}$  in  $A$ .

Both  $F_1$  and  $F_2$  are defined up to multiplication by a common orthogonal  $r \times r$  matrix from the left, and therefore, the generalized Schur complement is well-defined and does not depend on the choice of  $F_1$ .

We then have the decomposition

$$(2.1) \quad A = P + B' = \begin{pmatrix} F_1^T \\ F_2^T \end{pmatrix} \begin{pmatrix} F_1^T \\ F_2^T \end{pmatrix}^T + \begin{pmatrix} B & 0 \\ 0 & 0 \end{pmatrix}$$

of  $A$  into a rank  $r$  positive semi-definite matrix  $P$  and a remainder  $B'$  which makes the generalized Schur complement appear in its upper left sub-block, its other blocks being zero.

LEMMA 2.10. *Assume above conditions and notations. Let  $v \in \mathbb{R}^n$  be orthogonal to the last  $n_2$  rows of  $P$ . Then  $v \in \ker P$ .*

*Proof.* By assumption, we have  $F_2^T (F_1 \ F_2) v = 0$ . But  $F_2$  has full row rank, and hence,  $(F_1 \ F_2) v = 0$ . It follows that also  $F_1^T (F_1 \ F_2) v = 0$ , and as a consequence  $Pv = 0$ .  $\square$

The following lemma is a consequence of the Albert nonnegative definiteness conditions [1].

LEMMA 2.11. *Assume above conditions and notations. If  $A$  is positive semi-definite, then also the generalized Schur complement  $B$  is positive semi-definite.*

**3. Main result.** First we shall extend Theorem 2.5 to the cases  $k = 3, 4$ .

LEMMA 3.1. *Theorem 2.5 holds also if  $k = 3$  or  $k = 4$ .*

*Proof.* Assume the notations in the formulation of Theorem 2.5, and suppose that either  $k = 3$  or  $k = 4$ . Let us first prove the implication (i)  $\Rightarrow$  (ii). Assume (i). By Lemma 2.1, we have that  $B_{I'_j} \succeq 0$ , and by Lemma 2.3, we have  $Bv^j \geq 0$ . Hence,  $(v^i)^T Bv^j \geq 0$  for all  $i, j = 1, \dots, k$ , implying (ii). Let us now prove the converse implication.

For  $k = 3$  we have  $I'_1 = \{3\}$ ,  $I'_2 = \{1\}$ ,  $I'_3 = \{2\}$ . The zeros  $v^j$  can then be chosen equal to the basis vectors of  $\mathbb{R}^3$ . The conditions of Theorem 2.5 imply  $\text{diag } B = \mathbf{0}$ . Moreover, we have  $(v^3)^T Bv^1 = B_{23}$ ,  $(v^1)^T Bv^2 = B_{13}$ ,  $(v^2)^T Bv^3 = B_{12}$ . The assertion of Theorem 2.5 reduces to the equivalence of the conditions

- (i)  $B \in \mathcal{C}^3$ ;
- (ii)  $B_{ij} \geq 0$  for all  $i, j = 1, \dots, 3$ .

The implication (ii)  $\Rightarrow$  (i) is now evident.

For  $k = 4$  we have  $I'_1 = \{3, 4\}$ ,  $I'_2 = \{4, 1\}$ ,  $I'_3 = \{1, 2\}$ ,  $I'_4 = \{2, 3\}$ . Assume (ii). Since  $B_{I'_j} \succeq 0$  for all  $j = 1, \dots, 4$ , we have in particular that  $\text{diag } B \geq 0$ . Hence,  $B_{jj} = d_j^2$  for some nonnegative  $d_j$ ,  $j = 1, \dots, 4$ . Moreover,  $B_{I'_j} \succeq 0$  and  $(v^j)^T Bv^j = (v^j)^T_{I'_j} B_{I'_j} v^j_{I'_j} = 0$  together imply  $B_{I'_j} v^j_{I'_j} = 0$  for all  $j = 1, \dots, 4$ . In particular,  $\det B_{I'_j} = 0$ , which implies  $B_{j,j+1} = \pm d_j d_{j+1}$ ,  $j = 1, 2, 3$ , and  $B_{14} = \pm d_1 d_4$ . If one of these off-diagonal elements of  $B$  is positive, then the corresponding product  $(v^j)^T Bv^j$  must also be positive by the positivity of  $v^j_{I'_j}$ . Hence, we have  $B_{j,j+1} = -d_j d_{j+1}$ ,  $j = 1, 2, 3$ ,  $B_{14} = -d_1 d_4$ .

Let  $v^3 = (\alpha, \beta, 0, 0)^T$  with  $\alpha > 0$ ,  $\beta > 0$ . Condition  $(v^3)^T Bv^3 = 0$  can then be written as  $\alpha^2 d_1^2 - 2\alpha\beta d_1 d_2 + \beta^2 d_2^2 = (\alpha d_1 - \beta d_2)^2 = 0$ . This implies  $\alpha d_1 = \beta d_2$ . In a similar way, let  $v^4 = (0, \gamma, \delta, 0)^T$  with  $\gamma > 0$ ,  $\delta > 0$ , we then get  $\gamma d_2 = \delta d_3$ . The condition  $(v^3)^T Bv^4 \geq 0$  then can be written as  $-\alpha\gamma d_1 d_2 + \alpha\delta B_{13} + \beta\gamma d_2^2 - \beta\delta d_2 d_3 \geq 0$ . Equivalently we obtain  $\alpha\delta(B_{13} - d_1 d_3) \geq -\alpha\delta d_1 d_3 + \alpha\gamma d_1 d_2 + \beta\delta d_2 d_3 - \beta\gamma d_2^2 = (\alpha d_1 - \beta d_2)(\gamma d_2 - \delta d_3) = 0$ , implying  $N_{13} = B_{13} - d_1 d_3 \geq 0$ . In an analogous manner we obtain  $N_{24} = B_{24} - d_2 d_4 \geq 0$ . This yields

$$B = \begin{pmatrix} d_1 \\ -d_2 \\ d_3 \\ -d_4 \end{pmatrix} \begin{pmatrix} d_1 \\ -d_2 \\ d_3 \\ -d_4 \end{pmatrix}^T + \begin{pmatrix} 0 & 0 & N_{13} & 0 \\ 0 & 0 & 0 & N_{24} \\ N_{13} & 0 & 0 & 0 \\ 0 & N_{24} & 0 & 0 \end{pmatrix},$$

and  $B$  can be decomposed into a sum of a matrix in  $\mathcal{S}_+^4$  and a matrix in  $\mathcal{N}^4$ . This implies  $B \in \mathcal{C}^4$ , completing the proof.  $\square$

**LEMMA 3.2.** Assume the notations of the previous section. Let  $3 \leq k \leq n - 1$  and let  $A \in \mathcal{C}^n$  have zeros with supports  $I_1, \dots, I_k$ . Then the submatrix  $A_{I_0}$  is positive semi-definite. If  $v \in \mathbb{R}^{n-k}$  is a kernel vector of  $A_{I_0}$ , then  $v' = (0, \dots, 0, v^T)^T \in \mathbb{R}^n$  is a kernel vector of  $A$ , where  $v'$  is obtained from  $v$  by appending  $k$  zeros at the beginning.

*Proof.* By Lemma 2.1, the submatrices  $A_{I_1}, \dots, A_{I_k}$  are positive semi-definite. It follows that  $A_{I_0}$  is also positive semi-definite, because it is a principal submatrix of  $A_{I_j}$  for all  $j = 1, \dots, k$ .

Let now  $v \in \mathbb{R}^{n-k}$  be a kernel vector of  $A_{I_0}$  and construct  $v' \in \mathbb{R}^n$  as in the statement of the lemma. Let also  $w \in \mathbb{R}^{n-2}$  be the vector obtained by appending  $k - 2$  zeros at the beginning of  $v$ . Let  $j \in \{1, \dots, k\}$  be arbitrary, and consider the submatrix  $A_{I_j}$ . Then  $w^T A_{I_j} w = v^T A_{I_0} v = 0$ . But  $A_{I_j} \succeq 0$ , hence, also  $A_{I_j} w = 0$ . Now  $A_{I_j} w = (Av')_{I_j}$ , and hence,  $(Av')_{I_j} = 0$  for all  $j = 1, \dots, k$ . However,  $\bigcup_{j=1}^k I_j = \{1, \dots, n\}$ , and therefore,  $Av' = 0$  as claimed.  $\square$

By Lemma 3.2, the matrix  $A$  satisfies the assumptions needed for the definition of the generalized Schur complement. Let  $B \in \mathcal{S}^k$  be the generalized Schur complement of  $A_{I_0}$  in  $A$ , and denote by  $r$  the rank of  $A_{I_0}$ . By (2.1),  $A$  can be decomposed into a sum

$$(3.2) \quad A = P + B', \quad B' = \begin{pmatrix} B & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix},$$

where  $P$  is a positive semi-definite matrix of rank  $r$ .

LEMMA 3.3. *Assume above notations. Then for all  $j = 1, \dots, k$ , we have  $Pu^j = 0$ .*

Recall that  $u^j$  is a zero of  $A$  with support  $I_j$ ,  $j = 1, \dots, k$ .

*Proof.* We have  $(Au^j)_{I_j} = 0$  by Lemma 2.2. Since  $I_0 \subset I_j$ , we get also  $(Au^j)_{I_0} = 0$ . Hence, the last  $n - k$  rows of  $A$  are orthogonal to  $u^j$ .

The last  $n - k$  rows of  $A$  coincide with the last  $n - k$  rows of  $P$ . Thus, also the last  $n - k$  rows of  $P$  are orthogonal to  $u^j$ . The assertion of the lemma now follows from Lemma 2.10.  $\square$

LEMMA 3.4. *Assume above notations. The generalized Schur complement  $B$  is copositive.*

*Proof.* We shall show that  $B$  satisfies conditions (ii) of Theorem 2.5.

Let us note  $v^j = (u^j)_{\bar{I}_0}$  for  $j = 1, \dots, k$ . Then by Lemma 3.3, we have  $0 = (u^j)^T Au^j = (u^j)^T Pu^j + (u^j)^T B'u^j = (v^j)^T Bv^j$  for all  $j = 1, \dots, k$ . Further, we get  $Au^j = B'u^j \geq 0$  by Lemmas 3.3 and 2.3, and hence,  $(B'u^j)_{\bar{I}_0} = Bv^j \geq 0$ . The inequality  $v^i \geq 0$  then yields  $(v^i)^T Bv^j \geq 0$  for all  $i, j = 1, \dots, k$ . Note also that  $\text{supp } v^j = I'_j$ ,  $j = 1, \dots, k$ . The submatrix  $B_{I'_j}$  is the Schur complement of  $A_{I_0}$  in the positive semi-definite matrix  $A_{I_j}$ . Hence,  $B_{I'_j} \succeq 0$  by Lemma 2.11.

Hence, the conditions (ii) of Theorem 2.5 are satisfied, and  $B \in \mathcal{C}^k$  by Theorem 2.5 for  $k \geq 5$  and by Lemma 3.1 for  $k = 3, 4$ .  $\square$

We are now able to prove our main result.

THEOREM 3.5. *Let  $A \in \mathcal{C}^n$  be an exceptional extremal copositive matrix. Let  $G$  be the graph on  $n$  vertices which has an edge  $(i, j)$  if and only if  $A$  has a zero with support  $\{1, \dots, n\} \setminus \{i, j\}$ . Suppose  $G$  contains a cycle of length  $k$  on the vertex subset  $I = \{i_1, \dots, i_k\}$ . Then all non-zero elements of  $A$  are contained in the submatrix  $A_I$ .*

*Proof.* If  $k = n$ , then there is nothing to prove.

Suppose  $3 \leq k \leq n - 1$ . Without loss of generality we may assume  $i_j = j$ ,  $j = 1, \dots, k$ , and adopt the notations above. In particular, the subset  $I$  then equals  $\bar{I}_0$ .

Consider decomposition (3.2). By Lemma 3.4, the matrix  $B$ , and hence, also the matrix  $B'$  is copositive. Hence,  $A$  has been represented as a sum of a positive semi-definite and a copositive matrix. Since  $A$  is extremal, these two matrices have to be proportional.

If  $P$  is a multiple of  $B'$ , then  $A$  is a multiple of  $B'$ , and the assertion of the theorem holds.

Suppose that  $P$  is not a multiple of  $B'$ . Then  $B' = 0$ , because  $P$  and  $B'$  are proportional. This implies  $A = P \succeq 0$ , contradicting the exceptionality of  $A$ . This completes the proof.  $\square$

We shall now deduce a number of consequences from Theorem 3.5.

**COROLLARY 3.6.** *Let  $A \in \mathcal{C}^n$  be an exceptional extremal copositive matrix with positive diagonal, and let  $G$  be the graph defined in Theorem 3.5. Then  $G$  does not contain any cycle of length strictly smaller than  $n$ . In particular, either  $G$  is the cycle graph  $C_n$ , or  $G$  is acyclic (i.e., a forest).*

*Proof.* Since all diagonal elements of  $A$  are positive, there exists no proper subset  $I \subset \{1, \dots, n\}$  such that all non-zero elements of  $A$  are contained in the submatrix  $A_I$ . The claim of the corollary then follows from Theorem 3.5.  $\square$

**COROLLARY 3.7.** *Let  $A \in \mathcal{C}^n$  be an exceptional extremal copositive matrix. Let  $G_{\min}$  be the graph on  $n$  vertices such that  $G_{\min}$  has an edge  $(i, j)$  if and only if there exists a minimal zero of  $A$  with support  $\{1, \dots, n\} \setminus \{i, j\}$ . Then  $G_{\min}$  cannot contain a cycle of length strictly smaller than  $n$ .*

*Proof.* For the sake of contradiction, suppose that  $G_{\min}$  contains a cycle  $C$  of length  $k < n$ . Let  $I \subset \{1, \dots, n\}$  be the subset of vertex indices in the cycle, then  $\bar{I} \neq \emptyset$ . By Theorem 3.5, all non-zero entries of  $A$  are contained in the submatrix  $A_I \in \mathcal{C}^k$ .

Let now  $(i, j)$  be an edge in the cycle  $C$  and  $u$  a minimal zero of  $A$  with support  $\{1, \dots, n\} \setminus \{i, j\}$ . Since  $i, j \in I$ , we have  $\bar{I} \subset \text{supp } u$ . On the other hand,  $\text{supp } u \cap I \neq \emptyset$ , because the cycle  $C$  has length at least 3. Consider the vector  $v \in \mathbb{R}^n$  defined element-wise by

$$v_l = \begin{cases} u_l, & l \in I, \\ 0, & l \notin I. \end{cases}$$

This vector is also a zero of  $A$ , and  $\text{supp } v \subset \text{supp } u$ . Since  $u$  is a minimal zero, we must have  $\text{supp } u = \text{supp } v \subset I$ , leading to a contradiction with the inclusion  $\bar{I} \subset \text{supp } u$ . This completes the proof.  $\square$

**COROLLARY 3.8.** *Let  $A \in \mathcal{C}^n$  be an exceptional extremal copositive matrix. Suppose all minimal zeros of  $A$  have supports of cardinality  $n - 2$ . Let  $G_{\min}$  be the graph defined in Corollary 3.7, and  $G$  the graph defined in Theorem 3.5. Then  $G_{\min}$  and  $G$  coincide and equal the cycle graph  $C_n$ .*

*Proof.* Assume the notations of the corollary. First we show that no three edges of  $G_{\min}$  can meet in the same vertex. For the sake of contradiction, let  $i, j, k$  be distinct vertices such that  $(i, k)$  and  $(i, j)$  are edges of  $G_{\min}$ . Then there exist minimal zeros  $u, v$  of  $A$  with supports  $I = \{1, \dots, n\} \setminus \{i, k\}$  and  $J = \{1, \dots, n\} \setminus \{i, j\}$ , respectively. We have  $J \setminus I = \{k\}$ , and these minimal zeros satisfy the conditions of Lemma 2.7. Hence, there are no minimal zeros  $w$  of  $A$  other than the multiples of  $u$  or  $v$  which have a support satisfying  $\text{supp } w \subset \{1, \dots, n\} \setminus \{i\}$ . This means  $G_{\min}$  cannot have an edge  $(i, l)$  with  $l \notin \{j, k\}$ , proving our claim.

On the other hand, by Lemma 2.8, there must be at least  $n$  linearly independent minimal zeros of  $A$ , which by Lemma 2.6 correspond to at least  $n$  distinct edges of  $G_{\min}$ . However, by the Dirichlet principle, a graph with  $n$  vertices and at least  $n$  edges such that at most two edges join in each vertex must contain exactly  $n$  edges such that there are exactly two edges joining at each vertex. Thus,  $G_{\min}$  is a disjoint union of cycles.

By Corollary 3.7, no cycle can have a length strictly smaller than  $n$ . Thus,  $G_{\min}$  is the cycle graph  $C_n$ .

Now by Lemma 2.4, the zero supports of  $A$  have cardinality at most  $n - 2$ . On the other hand, no zero can have a support of cardinality strictly less than  $n - 2$ , because there are no minimal zeros with such supports. It follows that every zero of  $A$  is also a minimal zero, and the graphs  $G_{\min}$  and  $G$  coincide. This concludes the proof.  $\square$

Copositive matrices such that the graph  $G$  defined in Theorem 3.5 or the graph  $G_{\min}$  defined in Corollary 3.7 is the cycle graph  $C_n$  have been studied in [11]. Therefore, the classification of all exceptional extremal copositive matrices such that all their minimal zeros have supports of cardinality  $n - 2$  reduces to the cases considered in [11].

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