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EXTREME VECTORS OF DOUBLY NONNEGATIVE MATRICES

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ABSTRACT. An $n \times n$ real symmetric matrix is *doubly nonnegative* if it is positive semi-definite and entrywise nonnegative. It is easy to check that the collection of all $n \times n$ doubly nonnegative matrices forms a closed convex cone. A vector lying on an extreme ray of this cone is referred to as an extreme DN matrix. In this note we obtain characterizations of extreme DN matrices and show that there exist $n \times n$ extreme DN matrices with rank k if and only if $k \neq 2$ and

$$k \leq \begin{cases} \max\{1, n-3\} & \text{if } n \text{ is even,} \\ \max\{1, n-2\} & \text{if } n \text{ is odd.} \end{cases}$$

Using these results, we obtain an algorithm for checking whether a given DN matrix is extreme. Some other results concerning extreme DN matrices are also proved.

1. Introduction. Let $S_n(\mathbf{R})$ be the linear space of $n \times n$ real symmetric matrices. A positive semi-definite matrix $A \in S_n(\mathbf{R})$ with all $A_{ij} \geq 0$ (entrywise nonnegative) is called a *doubly nonnegative matrix.* A positive semi-definite matrix $A = XX^t \in S_n(\mathbf{R})$ with $X \geq 0$ (entrywise) is called a *completely positive matrix.* Denote by DN and CP the set of doubly nonnegative matrices and the set of completely positive matrices, respectively. Evidently, $CP \subseteq DN$, and it is known (e.g., see [**7**]) that the two sets are equal if and only if $n \leq 4$.

It is clear that both DN and CP are closed convex cones. There has been a great deal of interest in studying these two cones (e.g., see [**1, 2, 3, 4, 5, 6, 7**] and their references) motivated by the study of various subjects such as M-matrices, graph theory, block designs in

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combinatorics, the theory of inequalities, statistics in the context of association in random vectors, and quadratic differential equations.

Recall that (e.g., see [**8**, Section 18]) an element x in a convex cone $\mathcal{K}$ is an *extreme vector* if it is not the midpoint of two other elements in the cone $\mathcal{K}$ that are not multiples of x, or equivalently, if it lies on an extreme ray of the cone. It is well known that every closed convex cone is generated by its extreme vectors, i.e., every element in the cone can be expressed as a convex combination of extreme vectors. Thus, it is helpful in understanding the structure of the cone if we know its extreme vectors. We shall denote the set of extreme vectors of a given closed convex cone $\mathcal{K}$ by $\text{Ext}\,(\mathcal{K})$.

Since CP is a subset of the convex hull of $\mathcal{S} = \{xx^t : x \in \mathbf{R}^n, x \geq 0 \text{ (entrywise)}\}$, it follows that $\text{Ext}\,(CP) \subseteq \mathcal{S}$. Moreover, if $A \in \mathcal{S}$, then $A \neq (B+C)/2$ for any $B, C \in CP$ that are not multiples of A. Hence, we conclude that $\text{Ext}\,(CP) = \mathcal{S}$.

The structure of $\text{Ext}\,(DN)$ seems more complicated. The purpose of this paper is to study $\text{Ext}\,(DN)$. We shall call $A \in \text{Ext}\,(DN)$ an *extreme DN matrix*. In Section 2, we give several characteristics of extreme DN matrices. The result is then used to design an algorithm to check whether a given DN matrix is extreme. Some other results on extreme DN matrices are also discussed. In Section 3 we show that there exist $n \times n$ extreme DN matrices with rank k if and only if $k \neq 2$ and

$$k \leq \begin{cases} \max\{1, n-3\} & \text{if } n \text{ is even,} \\ \max\{1, n-2\} & \text{if } n \text{ is odd.} \end{cases}$$

In particular, we provide constructions for extreme DN matrices of different ranks. We also show that if $n \geq 5$ is odd and $A \in DN$ has rank $n-2$, then $A \in \text{Ext}\,(DN)$ if and only if the graph of A (see the definition in Section 3) is a cycle of length n. From these results, one easily deduces that $CP = DN$ if $n \leq 4$ (see Corollary 3.3). Some remarks and related problems are mentioned in Section 4. Some of our results have also been obtained in [**9**] by different methods. Our approach seems to be more elementary.

In our discussion, we use $\{e_1, \ldots, e_n\}$ to denote the standard basis of $\mathbf{R}^n$, and use $\{E_{11}, E_{12}, \ldots, E_{nn}\}$ to denote the standard basis of $n \times n$ real matrices. The usual inner product on $S_n(\mathbf{R})$ is defined and denoted by $\langle A, B \rangle := \text{tr}\ (AB)$.

2. Characteristics and an algorithm. Suppose $A \in DN$ is nonzero. It is not hard to see that $A \in DN$ is not extreme if and only if there exists a matrix $P \in S_n(\mathbf{R})$ not equal to a multiple of A such that $A \pm \varepsilon P$ are DN matrices for sufficiently small $\varepsilon > 0$. In fact, if $A = (B + C)/2$ with $B, C \in DN$ such that B and C are not multiples of A, then $P = (P - B)/2$ is such a matrix; if P is a matrix satisfying the said conditions, then $A = (B + C)/2$ with $B = A + \varepsilon P$, $C = A - \varepsilon P \in DN$ for some sufficiently small $\varepsilon > 0$. We shall call the matrix P with the said properties a *perturbation* of A. In the following theorem, we give a characterization of perturbations of a given $A \in DN$ and use it to determine whether $A \in \operatorname{Ext}(DN)$.

Theorem 2.1. *Suppose $A \in DN$ has rank $k \geq 1$ and $A = XX^t$ for some $X \in \mathbf{R}^{n\times k}$. Let*

$$W_1 = \{XQX^t : Q \in S_k(\mathbf{R})\}, \qquad W_2 = \{Y : Y_{ij} = 0 \text{ if } A_{ij} = 0\},$$

and

$$\mathcal{B} = \{E_{ij} + E_{ji} : A_{ij} = 0\}.$$

Then a matrix P is a perturbation of A if and only if $P \in W_1 \cap W_2$ and P is not a multiple of A. Consequently, $A \in \operatorname{Ext}(DN)$ if and only if any one of the following conditions holds.

(a) $W_1 \cap W_2 = \{\lambda A : \lambda \in \mathbf{R}\}$.

(b) $\operatorname{span}\{X^tRX : R \in \mathcal{B}\} = \{I_k\}^\perp$ *in* $S_k(\mathbf{R})$.

(c) $\operatorname{span}\{X^tRX : R \in \mathcal{B}\}$ *has dimension* $k(k+1)2 - 1$.

Proof. If P is a perturbation of A, then P is not a multiple of A. Since $A \pm \varepsilon P$ is positive semi-definite for sufficiently small $\varepsilon > 0$, the range space of P is contained in that of A. Thus $P \in W_1$. Since $A \pm \varepsilon P$ has nonnegative entries, $P \in W_2$.

Conversely, suppose $P = XQX^t \in W_1 \cap W_2$ is not a multiple of A. Then, for sufficiently small $\varepsilon > 0$, $I_k \pm \varepsilon Q$ are positive semi-definite and $A \pm \varepsilon P$ has nonnegative entries. Thus, P is a perturbation of A.

Now if $A \in \operatorname{Ext}(DN)$, then it has no perturbations. Thus, every $P \in W_1 \cap W_2$ is a multiple of A, and condition (a) holds.

Suppose that condition (a) holds. With the notation of the theorem, one sees that $\mathcal{B}$ is a basis for $W_2^\perp$. Since $0 = \langle A, R\rangle = \langle I_k, X^tRX\rangle$

for all $R \in \mathcal{B}$, we see that $I_k \in \{X^tRX : R \in \mathcal{B}\}^\perp$. Suppose $Q \in \{X^tRX : R \in \mathcal{B}\}^\perp$. Then $0 = \langle Q, X^tRX\rangle = \langle XQX^t, R\rangle$ for all $R \in \mathcal{B}$. Thus, $XQX^t \in (W_2^\perp)^\perp = W_2$. Since $XQX^t \in W_1$, it follows from condition (a) that $XQX^t = \lambda A$ for some $\lambda \in \mathbf{R}$. Since X has full column rank, we conclude that $Q = \lambda I_k$. Thus, $\{X^tRX : R \in \mathcal{B}\}^\perp = \{\lambda I_k : \lambda \in \mathbf{R}\}$ and condition (b) follows.

It is clear from the previous discussion that $I_k \in \{X^tRX : R \in \mathcal{B}\}^\perp$. One easily sees that conditions (b) and (c) are equivalent.

Finally, suppose that (b) holds. If $A \notin \mathrm{Ext}\,(DN)$, then there exists a perturbation $P = XQX^t \neq \lambda A$ in $W_1 \cap W_2$. Note that $Q \neq \lambda I_k$ as $P \neq \lambda A$. Since $\mathcal{B} \subseteq W_2^\perp$, $0 = \langle XQX^t, R\rangle = \langle Q, X^tRX\rangle$ for all $R \in \mathcal{B}$. Thus, $Q \in \{X^tRX : R \in \mathcal{B}\}^\perp \neq \mathrm{span}\,\{I_k\}$, which is a contradiction. □

By Theorem 2.1, we have the following necessary condition for extreme DN matrices.

Corollary 2.2. *Let $A \in \mathrm{Ext}\,(DN)$ have rank $k \geq 1$. Then there are at least $k(k+1)/2 - 1$ entries in the upper triangular part of A equal to zero.*

Proof. Let X and $\mathcal{B}$ satisfy the hypotheses of Theorem 2.1. Since $A \in \mathrm{Ext}\,(DN)$, $\mathrm{span}\,\{X^tRX : R \in \mathcal{B}\} = \{I_k\}^\perp$ has dimension $k(k+1)/2 - 1$, and hence there are at least $k(k+1)2 - 1$ elements in $\mathcal{B}$. □

Before continuing our discussion, we make several observations that are useful in our study.

(i) If $A = XX^t$ as stated in Theorem 2.1, where X^t has columns $v_1, \ldots, v_n \in \mathbf{R}^k$, and if $A_{ij} = 0$, then $X^t(E_{ij} + E_{ji})X$ is of the form $v_iv_j^t + v_jv_i^t$.

(ii) If $A \in DN$ and P is a permutation matrix, then $A \in \mathrm{Ext}\,(DN)$ if and only if $P^tAP \in \mathrm{Ext}\,(DN)$.

(iii) If $A \in CP$, then $A \in \mathrm{Ext}\,(DN)$ if and only if A has rank 1.

We are now ready to consider some other consequences of Theorem

2.1. In particular, the following results show that one can determine whether $A \in \text{Ext}\,(DN)$ by studying the principal submatrices of A.

Proposition 2.3. *Suppose that $\hat{A}$ is a principal submatrix of A such that the* $\text{rank}\,(\hat{A}) = \text{rank}\,(A) = k \geq 1$. *If $\hat{A} \in \text{Ext}\,(DN)$ (in the lower dimensional case), then $A \in \text{Ext}\,(DN)$.*

Proof. By observation (ii), we may assume that $\hat{A} \in S_m(\mathbf{R})$ is the leading principal submatrix of A. Suppose that $A = XX^t$, where X is an $n \times k$ matrix and X^t has columns $v_1, \dots, v_n$. Then $\hat{A} = YY^t$, where Y^t has columns $v_1, \dots, v_m$. Since $\hat{A} \in \text{Ext}\,(DN)$, we have $\{I_k\}^\perp = \text{span}\,\{v_i v_j^t + v_j v_i^t : \hat{A}_{ij} = 0\} \subseteq \text{span}\,\{v_i v_j^t + v_j v_i^t : A_{ij} = 0\}$. It follows that $A \in \text{Ext}\,(DN)$. □

Proposition 2.4. *Suppose that $A \in DN$ is nonzero and is permutationally similar to $A_1 \oplus A_2$. Then $A \in \text{Ext}\,(DN)$ if and only if A_1 or $A_2 = 0$ and the nonzero A_i is an extreme DN matrix (in the lower dimension case).*

Proof. By observation (ii), we may assume that $A = A_1 \oplus A_2$.

Suppose $A \in \text{Ext}\,(DN)$. If none of A_1 and A_2 are zero, then $B = 2A_1 \oplus 0$ and $C = 0 \oplus 2A_2$ are DN matrices not equal to multiples of A such that $A = (B+C)/2$, which is a contradiction. So we may assume that $A = A_1 \oplus 0$ with $A_1 \in S_m(\mathbf{R})$ such that $\text{rank}\, A = \text{rank}\, A_1 = k$. Suppose that $A = XX^t$ as in Theorem 2.1, and X^t has columns $v_1, \dots, v_m, 0, \dots, 0$. Then $\{I_k\}^\perp = \text{span}\,\{v_i v_j^t + v_j v_i^t : A_{ij} = 0\} = \text{span}\,\{v_i v_j^t + v_j v_i^t : (A_1)_{ij} = 0\}$. It follows that $A_1 \in \text{Ext}\,(DN)$.

The converse follows easily from Proposition 2.3. □

Corollary 2.5. *If there exists a rank k extreme DN matrix in $S_n(\mathbf{R})$, then for any $m \geq n$ there exist rank k extreme DN matrices in $S_m(\mathbf{R})$.*

Proof. If $A \in \text{Ext}\,(DN)$ is $n \times n$ and has rank k, then $A \oplus 0_{m-n} \in \text{Ext}\,(DN)$ for any $m \geq n$. □

We shall give complete information about the rank restrictions on extreme DN matrices in the next section. We conclude this section with the following algorithm for checking whether a matrix $A \in DN$ is extreme.

Algorithm for checking extreme DN matrices. *Suppose $A \in DN$ is nonzero.*

Step 1. *Determine the rank of A.*

Step 2. *Write A as XX^t for an $n \times k$ matrix X, where k is the rank of A.*

Step 3. *Determine the dimension d of* span $\{X^t(E_{ij} + E_{ji})X : i \leq j, A_{ij} = 0\}$.

Then $d = k(k+1)/2 - 1$ if and only if $A \in \text{Ext}\,(DN)$.

To determine the value d in Step 3, let $\{X^t(E_{ij} + E_{ji})X : i \leq j, A_{ij} = 0\} = \{C_1, \dots, C_m\}$. For instance, one can use Observation (i) to construct $C_1, \dots, C_m$. Next, construct the $m \times k(k+1)/2$ matrix $\mathbf{C}$ such that the jth row of $\mathbf{C}$ is the coordinate vector of the matrix C_j with respect to the basis

$$\{E_{rr} \in S_k(\mathbf{R}) : 1 \leq r \leq k\} \cup \{E_{rs} + E_{sr} \in S_k(\mathbf{R}) : 1 \leq r < s \leq k\}$$

for $S_k(\mathbf{R})$, i.e., the jth row of $\mathbf{C}$ contains the entries of C_j in its upper triangular part. Then d is just the rank of the matrix $\mathbf{C}$.

3. Rank restrictions on extreme DN matrices. To study the rank restrictions on extreme DN matrices, we need the concept of the graph of a matrix. For a given $A \in S_n(\mathbf{R})$, let $G(A)$ denote the graph with n vertices, $\{1, \dots, n\}$ such that there exists an edge between two different vertices i and j if and only if $A_{ij} = A_{ji} \neq 0$.

The following additional observations are needed in our discussion.

(iv) If $A \in S_n(\mathbf{R})$ is positive semi-definite and if $A_{ii} = 0$, then the ith row (and also the ith column) is zero.

(v) A matrix $A \in S_n(\mathbf{R})$ is reducible, i.e., A is permutationally similar to the direct sum of matrices of lower orders, if and only if $G(A)$ is not connected.

(vi) If $A \in DN$ and $G(A)$ is a bipartite graph, then $A \in CP$. In particular, if such an A has rank larger than one, then A is the sum of more than one rank one CP matrix, and hence $A \notin \mathrm{Ext}\,(EN)$.

One may see [**1**] for the proof of observation (vi). The main results of this section are the following theorems.

Theorem 3.1. *There exists an $n \times n$ extreme DN matrix with rank $k \geq 1$ if and only if $k \neq 2$ and*

$$k \leq \begin{cases} \max\{1, n-3\} & \text{if } n \text{ is even} \\ \max\{1, n-2\} & \text{if } n \text{ is odd.} \end{cases}$$

Theorem 3.2. *Suppose that $n \leq 5$ is odd and $A \in DN$ has rank $n-2$. Then $A \in \mathrm{Ext}\,(DN)$ if and only if $G(A)$ is a cycle of length n.*

Since two closed convex cones are equal if and only if they have the same extreme vectors, one easily deduces the following corollary from Theorem 3.1.

Corollary 3.3. *If $n \leq 4$, $DN = CP$.*

The proof of Theorems 3.1 and 3.2 are divided into several lemmas. In particular, we exhibit a construction of rank k extreme DN matrices for those k satisfying the conditions in Theorem 3.1.

Lemma 3.4. *If $A \in \mathrm{Ext}\,(DN)$ has* rank k, *then $k \leq \max\{1, n-2\}$.*

Proof. Suppose that $A \in \mathrm{Ext}\,(DN)$ has rank $n > 1$. By Corollary 2.2, A has at least $n(n+1)/2 - 1$ zero entries in the upper triangular part. Since $A \neq 0$, there must be at least one nonzero entry. Since A is positive semi-definite, the nonzero entry must be on the diagonal. It follows that A has rank $1 < n$, which is a contradiction.

Suppose that $A \in \mathrm{Ext}\,(DN)$ has rank $n-1 > 1$. By Corollary 2.2, A has at least $n(n-1)/2 - 1$ zero entries, or equivalently, there are at most $n+1$ nonzero entries in the upper triangular part. Note that all diagonal entries of A are nonzero; otherwise, by observation (iv), A is permutationally similar to $A_1 \oplus [0]$. By Proposition 2.4, $A_1 \in S_{n-1}(\mathbf{R})$ is a rank $n-1$ extreme matrix, which contradicts the result established in the preceding paragraph. As a result, there is at most one nonzero entry in the strictly upper triangular part of A. Since $n \geq 3$, A is permutationally similar to $A_1 \oplus A_2$ for some $A_1 \in S_2(\mathbf{R})$ with both A_1 and A_2 nonzero. This contradicts Proposition 2.4. □

We remark that in the second part of the proof in the above lemma, once we see that there can only be one nonzero entry in the strict upper triangular part of A, we can conclude that $G(A)$ is bipartite, and hence $A \in \mathrm{Ext}\,(DN)$ by observation (vi).

Lemma 3.5. *Suppose that $n \geq 4$ and $A \in DN$ has* rank $n-2$. *If n is even, then $A \notin \mathrm{Ext}\,(DN)$. If n is odd and $A \in \mathrm{Ext}\,(DN)$, then $G(A)$ is a cycle of length n.*

Proof. Suppose that n and A satisfy the hypotheses of the lemma. If $A \in \mathrm{Ext}\,(DN)$, then Corollary 2.2 implies that there are at least $(n-1)(n-2)/2-1$ zero entries in the upper triangular part of A, i.e., there are at most $2n$ nonzero entries. Similar to the proof of Lemma 3.4, we can show that all diagonal entries of A are nonzero. Thus, there are at most n edges in $G(A)$. Furthermore, $G(A)$ is connected; otherwise, A is permutationally similar to $A_1 \oplus A_2$ by observation (v), and one of the A_i is zero by Proposition 2.4, which is a contradiction. Thus, $G(A)$ has at least $n-1$ edges.

If $G(A)$ has exactly $n-1$ edges, then $G(A)$ is a tree and hence a bipartite graph. By observation (vi), $A \notin \mathrm{Ext}\,(DN)$. Finally, suppose that $G(A)$ has n edges. We claim that every vertex of $G(A)$ has degree two, and hence $G(A)$ is a cycle. If it is note true, then $G(A)$ has a vertex of degree one. In the matrix A, it means that there is a row with exactly one nonzero off-diagonal entry. By observation (ii), we may assume that it is the first row, and $A_{12} \neq 0$. Suppose that $A = XX^t$ and $\mathcal{B}$ are defined as in Theorem 2.1. Let X have columns $v_1, \ldots, v_n \in \mathbf{R}^{n-2}$. Then $0 = A_{1j} = v_1 v_j^t$ for $j = 3, \ldots, n$. Since span $\{v_1, \ldots, v_n\}$ has dimension $n-2$ and $v_3, \ldots, v_n \in \{v_1\}^{\perp}$ in $\mathbf{R}^{n-2}$, it follows that $\{v_3, \ldots, v_n\}$ is linearly dependent. Note that if

$\sum_{i=3}^n \alpha_i v_i = 0$, then $\sum_{i=3}^n \alpha_i(v_1 v_i^t + v_i v_1^t) = 0$. Thus, $\{v_1 v_j^t + v_j v_1^t : j = 3, \ldots, n\} \subseteq \{X^t R X : R \in \mathcal{B}\}$ is linearly independent, and hence span $\{X^t R X : X \in \mathcal{B}\}$ has dimension strictly less than the number of elements in $\mathcal{B}$, which equals $(n-1)(n-2)/2 - 1$. By Theorem 2.1 (c), A cannot be a rank $n-2$ extreme DN matrix. Thus, our claim is proved, and $G(A)$ must be a cycle of length n. If n is even, then $G(A)$ is a bipartite graph, and hence $A \notin \text{Ext}\,(DN)$ by observation (vi). The conclusions follow. □

We are now ready to give the

Proof of Theorem 3.2. (⇒) by Lemma 3.5.

(⇐). Suppose that $A \in DN$ has rank $n-2$ and that $G(A)$ is a cycle of length n. By observation (ii), we may assume that $A_{ij} \neq 0$ if and only if $|i-j| \leq 1$ or $\{i,j\} = \{1,n\}$. We show that A has no perturbations, and hence is an extreme DN matrix. To achieve this end, let $A = XX^t$, W_1, W_2 and $\mathcal{B}$ be defined as in Theorem 2.1. Denote the columns of X^t by $v_1, \ldots, v_n \in \mathbf{R}^{n-2}$. Suppose $P = XQX^t \in W_2$ is a perturbation of A. We first show that $Qv_1 = \lambda_1 v_1$ for some $\lambda_1 \in \mathbf{R}$. Consider the zero pattern of the $n \times (n-2)$ matrix $\hat{A}$ obtained from A by removing its second and last columns. One easily sees that $\hat{A}$ has rank $n-2$. Since $\hat{A} = X\hat{X}^t$, where $\hat{X}^t$ is obtained from X^t by removing its second and last columns, it follows that $\hat{X}$ has rank $n-2$, and thus span $\{v_j : 1 \leq j \leq n-1, j \neq 2\} = \mathbf{R}^{n-2}$. By the fact that $0 = A_{1j} = v_1^t v_j$ for all j with $3 \leq j \leq n-1$, we conclude that $W = \text{span}\,\{v_j : 3 \leq j \leq n-1\} = \{v_1\}^\perp$. Now, since $0 = P_{1j} = v_1^t Q v_j$ for $j = 3, \ldots, n-1$, we see that $Q^t v_1 = Qv_1 \in W^\perp$. Thus, $Qv_1 = \lambda_1 v_1$ for some $\lambda_1 \in \mathbf{R}$ as asserted. One can use similar arguments to show that $Qv_j = \lambda_j v_j$ for some $\lambda_j \in \mathbf{R}$ for $j = 2, \ldots, n$.

To finish the proof, we show that all λ_i are equal, and hence $Q = \lambda_1 I$. Thus, $P = XQX^t = \lambda_1 A$, which contradicts the fact that P is a perturbation of A. To show that $\lambda_1 = \lambda_2$, recall that $\{v_j : 1 \leq j \leq n-1, j \neq 2\}$ is a basis of $\mathbf{R}^{n-2}$. Thus, $v_2 = \alpha_1 v_1 + \sum_{j=3}^{n-1} \alpha_j v_j$ for some $\alpha_i \in \mathbf{R}$. Since $0 \neq A_{12} = v_1^t v_2$, we conclude that $v_2 \notin \{v_1\}^\perp$, and hence $\alpha_1 \neq 0$. Now we also have $\lambda_2 v_2 = Qv_2 = \alpha_1 \lambda_1 v_1 + \sum_{i=3}^{n-1} \alpha_i \lambda_i v_i$. It follows that $\alpha_1 \lambda_1 = \alpha_1 \lambda_2$, and thus $\lambda_1 = \lambda_2$. One can use similar arguments to show that $\lambda_j = \lambda_{j+1}$ for $j = 2, \ldots, n-1$, and the desired conclusion follows. □

We need two more lemmas to complete the proof of Theorem 3.1.

Lemma 3.6. *If* $A \in \mathrm{Ext}\,(DN)$ *has rank* k*, then* $k \neq 2$.

Proof. Notice that by Lemmas 3.4 and 3.5, there is no rank two extreme DN matrix of size less than 5. Suppose that A is a rank two $n \times n$ extreme DN matrix, where $n \geq 5$. Let $A = XX^t$ and let $\mathcal{B}$ be defined as in Theorem 2.1. Suppose X^t has columns $v_1, \dots, v_n \in \mathbf{R}^2$. By Theorem 2.1, there exist $R_1 = E_{pq} + E_{qp}$, $R_2 = E_{rs} + E_{sr} \in \mathcal{B}$ such that span $\{X^t R_1 X, X^t R_2 X\} = \{I_2\}^{\perp}$. Let Y be the submatrix of X consisting of the rows in $\{v_p^t, v_q^t, v_r^t, v_s^t\}$. Then YY^t is a submatrix of A of size less than or equal to 4. By our construction, YY^t is an extreme DN matrix, which is a contradiction. □

To complete the proof of Theorem 3.1, we give a construction of rank k extreme DN matrices for those k satisfying the conditions in Theorem 3.1 in the following lemma.

Lemma 3.7. *Suppose that* k *satisfies the conditions in Theorem* 3.1. *There exist rank* k *extreme* DN *matrices.*

Proof. If $k = 1$, then, clearly, E_{11} is a rank 1 extreme DN matrix.

Construction for the case when $k \geq 3$ *is odd.* If $k \geq 3$ is odd, then $n \geq k+2$. By Proposition 2.4, it suffices to construct a $(k+2) \times (k+2)$ extreme DN matrix A. Then $A \oplus 0_{n-k-2}$ will be an $n \times n$ extreme DN matrix. To this end, let $A = XX^t$ be such that X^t has columns $v_1, \dots, v_{k+2} \in \mathbf{R}^k$, where $v_j = e_j + e_{j+1}$ for $j = 1, \dots, k-1$, $v_k = \sum_{j=1}^{k-1} (-1)^j e_j$, $v_{k+1} = v_k - e_k$, and $v_{k+2} = v_{k+1} + (k-1)e_1$, i.e.,

$$X = \underbrace{\begin{bmatrix} 1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 1 & 0 & \cdots & 0 \\ & & & \vdots & & \\ 0 & 0 & \cdots & 0 & 1 & 1 \\ -1 & 1 & -1 & \cdots & 1 & 0 \\ -1 & 1 & -1 & \cdots & 1 & -1 \\ k-2 & 1 & -1 & \cdots & 1 & -1 \end{bmatrix}}_{k \text{ columns}}$$

One can check that A has rank k and is of the form

$$\begin{bmatrix} 2 & 1 & 0 & \cdots & 0 & k-1 \\ 1 & \ddots & \ddots & \ddots & & 0 \\ 0 & \ddots & 2 & 1 & \ddots & \vdots \\ \vdots & \ddots & 1 & k-1 & k-1 & 0 \\ 0 & & \ddots & k-1 & k & 1 \\ k-1 & 0 & \cdots & 0 & 1 & k^2-3k+3 \end{bmatrix}.$$

Clearly $G(A)$ is a cycle of length $k+2$. By Theorem 3.2, $A \in \operatorname{Ext}(DN)$.

Construction for the case when $k \geq 4$ is even. If $k \geq 4$ is even, then $n \geq k+3$. Similar to the previous case, it suffices to construct a $(k+3) \times (k+3)$ extreme DN matrix A. To this end, let $A = XX^t$ be such that X^t has columns $v_1, \ldots, v_{k+3} \in \mathbf{R}^k$, where $v_j = e_j + e_{j+1}$ for $j = 1, \ldots, k-2$, $v_{k-1} = \sum_{j=1}^{k-2} (-1)^j e_j$, $v_k = v_{k-1} - e_{k-1}$, $v_{k+1} = v_k + (k-2)e_1$, $v_{k+2} = v_k + e_k$, and $v_{k+3} = v_{k+1} - e_k$, i.e.,

$$X = \underbrace{\left[\begin{array}{cccccc|c} 1 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 1 & 0 & \cdots & 0 & 0 \\ & & & \vdots & & & 0 \\ 0 & 0 & \cdots & 0 & 1 & 1 & \vdots \\ -1 & 1 & -1 & \cdots & 1 & 0 & \vdots \\ -1 & 1 & -1 & \cdots & 1 & -1 & \vdots \\ k-3 & 1 & -1 & \cdots & 1 & -1 & 0 \\ \hline -1 & 1 & -1 & \cdots & 1 & -1 & 1 \\ k-3 & 1 & -1 & \cdots & 1 & -1 & -1 \end{array}\right]}_{k \text{ columns}}$$

Note that the leading $(k+1)\times(k+1)$ principal submatrix of A is of the form YY^t, where the columns of Y^t are $v_1,\dots,v_{k+1}$. If we ignore the last zero entry of each $v_1,\dots,v_{k+1}$, they are constructed as in the odd rank case in the preceding paragraph. One easily checks that YY^t is an extreme DN matrix of rank $k-1$. Direct computation shows that the last two rows of A, i.e., the $(k+2)$nd and $(k+3)rd$ rows, are

$$(\underbrace{0,\dots,0}_{k-2},k-2,k-1,1,k,0),$$

$$(k-2,\underbrace{0,\dots,0}_{k-2},1,k^2-5k+4,0,k^2-5k+5).$$

Let $\mathcal{B}$ be defined as in Theorem 2.1. We claim that $\{X^tRX : R\in\mathcal{B}\}$ spans $\{I_k\}^\perp$, and hence $A\in \operatorname{Ext}(DN)$.

First we consider those $R=E_{ij}+E_{ji}\in\mathcal{B}$ with $1\le i,j\le k+1$. As mentioned before, the leading principal $(k+1)\times(k+1)$ submatrix of A is a rank $k-1$ extreme DN matrix. By our construction, such X^tRX will generate all matrices in $\{I_k\}^\perp$ whose last row and last column contain only zeros.

Next we show that there exist $Z_1,\dots,Z_k\in\{I_k\}^\perp$ (in $S_k(\mathbf{R})$) of the form X^tRX, where $R=E_{ij}+E_{ji}\in\mathcal{B}$ and $i\ge k+2$ or $j\ge k+2$, such that the last columns z_i of Z_i, $1\le i\le k$, form a basis of $\mathbf{R}^k$. Our assertion will then follow. Now, for $i=1,\dots,k-2$, let $Z_i=X^t(E_{i,k+2}+E_{k+2,i})X$. Then $z_i=e_i+e_{i+1}$. Next, let $Z_{k-1}=X^t(E_{k-1,k-3}+E_{k+3,k-1})X$ and $Z_k=X^t(E_{k+2,k+3}+E_{k+3,k+2})X$. Then $z_{k-1}=\sum_{i=1}^{k-2}(-1)^{i+1}e_i$ and $z_k=(k-2)e_1-2e_k$. One easily checks that $\{z_1,\dots,z_k\}$ is a basis for $\mathbf{R}^k$, and our result follows. □

4. Remarks and related problems. We remark that our techniques can be used to study extreme vectors of other convex sets or convex cones. In fact, we have proved some results of similar types on the convex sets obtained by intersecting DN or CP with the convex set of correlation matrices, i.e., positive semi-definite matrices in $S_n(\mathbf{R})$ with all diagonal entries equal to one.

Dr. B.S. Tam pointed out that our techniques can be extended to a more general cone theoretic scheme of relating the perturbation space, i.e., the linear space formed by perturbations and the zero vector, to a face of a convex cone.

Several problems related to our results are of interest. First, it would be nice to have a complete description or an algorithm to generate all extreme DN matrices. Also, it would be interesting to study other facial structures of the cones DN and CP. Another problem is to study the facial structures of the dual cones of DN and CP.

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