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On the nullspace, the rangespace and the characteristic polynomial of Euclidean distance matrices ☆

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Abstract

We present a characterization of the nullspace and the rangespace of a Euclidean distance matrix (EDM) D in terms of the vector of all ones, and in terms of the Gale subspace $G(D)$ and the realization matrix P corresponding to D. This characterization is then used to compute the characteristic polynomial of D. We also present some results concerning EDMs generated by regular figures and EDMs generated by centrally symmetric points.

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Keywords: Euclidean distance matrices; Gale transform; Characteristic polynomial

1. Introduction

An $n \times n$ matrix $D = (d_{ij})$ is called a *Euclidean distance matrix* (*EDM*) if there exist points $p^1, p^2, \ldots, p^n$ in some Euclidean space $\Re^r$ such that

$$d_{ij} = \|p^i - p^j\|^2 \quad \text{for all } i, j = 1, \ldots, n,$$

where $\|\|$ denotes the Euclidean norm. Let D be an EDM, the dimension of the affine span of the points $p^1, \ldots, p^n$ that generate D is called the *embedding dimension* of D. If the points $p^1, p^2, \ldots, p^n$ that generate an EDM D lie on a hypersphere, then D is called a *spherical EDM*. Otherwise, D is called *non-spherical*.

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Applications of EDMs include, among others, molecular conformation problems in chemistry [2], multidimensional scaling in statistics [7], and wireless sensor network localization problems [11].

Let $\mathscr{S}_n$ denote the set of symmetric real matrices of order n. We denote the nullspace and the rangespace of a matrix A by $N(A)$ and $R(A)$ respectively. I denotes the identity matrix of order n and e denotes the vector in $\Re^n$ of all ones. Finally, diag (A) denotes the vector consisting of the diagonal entries of a matrix A.

2. Preliminaries

Let $J := I - ee^{\mathrm{T}}/n$ denote the orthogonal projection on subspace $M := \{x \in \Re^n : e^{\mathrm{T}}x = 0\}$. It is well known [10] that a symmetric matrix D with zero diagonal is an EDM if and only if D is negative semidefinite on M. As a result, EDMs have exactly one positive eigenvalue. Let $\mathscr{S}_H = \{A \in \mathscr{S}_n : \mathrm{diag}\,(A) = 0\}$; and let $\mathscr{S}_C = \{A \in \mathscr{S}_n : Ae = 0\}$. Following [3], let $\mathscr{T} : \mathscr{S}_H \to \mathscr{S}_C$ and $\mathscr{K} : \mathscr{S}_C \to \mathscr{S}_H$ be the two linear maps defined by

$$\mathscr{T}(D) := -\frac{1}{2} JDJ, \tag{1}$$

$$\mathscr{K}(B) := \mathrm{diag}\,(B)e^{\mathrm{T}} + e(\mathrm{diag}\,(B))^{\mathrm{T}} - 2B. \tag{2}$$

Then it immediately follows that $\mathscr{T}$ and $\mathscr{K}$ are mutually inverse between the two subspaces $\mathscr{S}_H, \mathscr{S}_C$; and that D is an EDM of embedding dimension r if and only if the matrix $\mathscr{T}(D)$ is positive semidefinite of rank r [3].

Let D be a given EDM with embedding dimension r. Then the points $p^1, \ldots, p^n$ in $\Re^r$ that generate D can be determined as follows. Since the matrix $\mathscr{T}(D)$ is positive semidefinite of rank r, $\mathscr{T}(D)$ can be factorized as $\mathscr{T}(D) = PP^{\mathrm{T}}$ where P is an $n \times r$ matrix. Then, it can be shown that the points $p^1, \ldots, p^n$ are given by the rows of P. The matrix P is called a *realization* of D. Note that $P^{\mathrm{T}}e = 0$ since $\mathscr{T}(D)e = 0$; i.e., the origin coincides with the centroid of the points $p^1, \ldots, p^n$. Also note that P is not unique. For the purposes of this paper, we will assume in the sequel that P is given by

$$P = W\Lambda^{1/2}, \tag{3}$$

where Λ is the $r \times r$ diagonal matrix consisting of the positive eigenvalues of $\mathscr{T}(D)$; and W is the $n \times r$ matrix whose columns are an orthonormal set of the eigenvectors of $\mathscr{T}(D)$ corresponding to these positive eigenvalues.

Let D be a given EDM of embedding dimension r generated by the points $p^1, \ldots, p^n$ in $\Re^r$. Then $r \leqslant n - 1$. Consider the $(r+1) \times n$ matrix

$$\begin{bmatrix} P^{\mathrm{T}} \\ e^{\mathrm{T}} \end{bmatrix} = \begin{bmatrix} p^1 & p^2 & \cdots & p^n \\ 1 & 1 & \cdots & 1 \end{bmatrix}.$$

The *Gale subspace* corresponding to D, denoted by $G(D)$, is defined by

$$G(D) := \text{Nullspace of } \begin{bmatrix} P^{\mathrm{T}} \\ e^{\mathrm{T}} \end{bmatrix}. \tag{4}$$

Note that this subspace is uniquely determined by D since for any P, P' such that $\mathscr{T}(D) = PP^{\mathrm{T}} = P'P'^{\mathrm{T}}$, we have $\mathrm{N}(P^{\mathrm{T}}) = \mathrm{N}(P'^{\mathrm{T}}) = \mathrm{N}(\mathscr{T}(D))$. Let $\bar{r}$ denote the dimension of $G(D)$, then $\bar{r} = n - 1 - r$ where r is the embedding dimension of D. For $\bar{r} \geqslant 1$, let Z be the $n \times \bar{r}$ matrix, whose columns form a basis for $G(D)$. Z is called a *Gale matrix* corresponding to D; and the ith row of Z, considered as a vector in $\Re^{\bar{r}}$, is called a *Gale transform* of p^i. Gale transform is well known in the theory of polytopes [4].

The following lemma, first proved in [1], follows directly from (2).

Lemma 2.1. *Let D be a given EDM matrix and let Z be a Gale matrix corresponding to D. Then*

$$DZ = [\alpha_1 e \quad \alpha_2 e \quad \cdots \quad \alpha_{\bar{r}} e],$$

where $[\alpha_1 \quad \cdots \quad \alpha_{\bar{r}}] = (\operatorname{diag} \mathcal{T}(D))^{\mathrm{T}} Z.$

Lemma 2.2. *Let $D \neq 0$ be an EDM. Then $N(D) \subseteq G(D)$.*

Proof. Let $x \in N(D)$ and let $B = \mathcal{T}(D)$. Then since B is positive semidefinite and D is nonnegative, it follows from (1) that

$$0 \geqslant -2n^2 x^{\mathrm{T}} B x = e^{\mathrm{T}} D e (e^{\mathrm{T}} x)^2 \geqslant 0.$$

Thus $e^{\mathrm{T}} D e (e^{\mathrm{T}} x)^2 = 0$. Hence, $e^{\mathrm{T}} x = 0$ and $Bx = 0$ since $D \neq 0$. The result follows since $N(B) = N(P^{\mathrm{T}})$. □

Let $D \neq 0$ be an EDM. Then many well-known results follow from Lemma 2.2. First, $N(D) \subset N(\mathcal{T}(D))$, established in [12], follows directly since $G(D) \subset N(\mathcal{T}(D))$. Second, the well-known result $r + 1 \leqslant \operatorname{rank} D \leqslant r + 2$, where r is the embedding dimension of D also follows from Lemma 2.2 and (2).

Next we characterize the nullspace and the rangespace of an EDM D. This characterization depends on whether D is a spherical EDM or not. We discuss, first, the case of spherical EDMs.

3. The case of spherical EDMs

The following characterization of spherical EDMs is well known.

Lemma 3.1. *Let $D \neq 0$ be a given $n \times n$ EDM with embedding dimension r and let Z be a Gale matrix corresponding to D. Then the following statements are equivalent.*

1. *D is a spherical EDM.*
2. Rank $D = r + 1$.
3. *The matrix $\lambda e e^{\mathrm{T}} - D$ is positive semidefinite for some scalar λ.*
4. *$r = n - 1$ or $DZ = 0$.*

The equivalence of statements 1 and 3 was shown in [9], the equivalence of statements 1, 2 and 3 was shown in [5,12], and the equivalence of statements 3 and 4 was shown in [1]. The equivalence of statements 1 and 4 can be directly proved as follows. In [12] it is proven that an EDM D is spherical iff there exists a vector $a \in \Re^r$ such that

$$Pa = \frac{1}{2} J \operatorname{diag} \mathcal{T}(D), \tag{5}$$

where P is a realization of D, r is the embedding dimension of D and J is the orthogonal projection on the subspace $M = e^{\perp}$. In such a case, the points that generate D lie on a hypersphere whose center is a and whose radius is equal to $(a^{\mathrm{T}} a + e^{\mathrm{T}} D e / 2n^2)^{1/2}$. But (5) holds iff either

$r = n - 1$, i.e., $\bar{r} = 0$, or $J \operatorname{diag} \mathscr{T}(D)$ belongs to the nullspace of $\begin{bmatrix} Z^{\mathrm{T}} \\ e^{\mathrm{T}} \end{bmatrix}$ which is equivalent to $Z^{\mathrm{T}} \operatorname{diag} \mathscr{T}(D) = 0$. Hence, by Lemma 2.1, this is equivalent to $DZ = 0$.

Next we characterize the nullspace of D.

Theorem 3.1. *Let $D \neq 0$ be a spherical EDM. Then $N(D) = G(D)$.*

Proof. $N(D) \subseteq G(D)$ follows from Lemma 2.2. But since D is a spherical EDM we also have from Lemma 3.1 that $G(D) \subseteq N(D)$. Hence the result follows. □

The following is an immediate corollary of Theorem 3.1 and the definition of $G(D)$.

Corollary 3.1. *Let $D \neq 0$ be a spherical EDM and let P be a realization of D. Then $R(D) = R([P\ e])$.*

Note that for a spherical EDM D of embedding dimension r, $\dim N(D) = n - \operatorname{rank} D = n - 1 - r = \bar{r} = \dim G(D)$ and $\dim R(D) = r + 1 = \dim R([P\ e])$.

Now it follows from (2) and the definition of P in (3) that $P^{\mathrm{T}} D P = -2(P^{\mathrm{T}} P)^2 = -2\Lambda^2$, where Λ is the diagonal matrix consisting of the positive eigenvalues of $\mathscr{T}(D)$. Let $Q = [P\Lambda^{-1/2} \quad e/\sqrt{n}]$. Then the non-zero eigenvalues of D are the same as the eigenvalues of $Q^{\mathrm{T}} D Q$. But

$$Q^{\mathrm{T}} D Q = \begin{bmatrix} -2\Lambda & \frac{1}{\sqrt{n}} \Lambda^{-1/2} P^{\mathrm{T}} D e \\ \frac{1}{\sqrt{n}} e^{\mathrm{T}} D P \Lambda^{-1/2} & \frac{1}{n} e^{\mathrm{T}} D e \end{bmatrix}. \tag{6}$$

$Q^{\mathrm{T}} D Q$ as given in (6) is a *bordered diagonal* matrix. Thus, the characteristic polynomial of an $n \times n$ spherical EDM D is given by

$$p(\lambda) = \lambda^{n-r-1} \left[\left(\lambda - \frac{1}{n} e^{\mathrm{T}} D e \right) \prod_{i=1}^{r} (\lambda - a_i) - \sum_{i=1}^{r} b_i^2 \prod_{j=1, j \neq i}^{r} (\lambda - a_j) \right], \tag{7}$$

where r is the embedding dimension of D, a_i and b_i are the ith coordinates of the vectors $-2\operatorname{diag}(P^{\mathrm{T}} P) = -2 \operatorname{diag} \Lambda$, and $\frac{1}{\sqrt{n}} (P^{\mathrm{T}} P)^{-1/2} P^{\mathrm{T}} D e$ respectively. Recall that the characteristic polynomial of $-2\mathscr{T}(D)$ is $\lambda^{n-r} \prod_{i=1}^{r} (\lambda - a_i)$. Three remarks are in order here. First, the coefficient of λ^{n-1} in (7) is zero since trace $D = 0$. Second, if $b_{i_0} = 0$ for some i_0, $1 \leqslant i_0 \leqslant r$, then a_{i_0} is an eigenvalue of D. Third, if $b_i \neq 0$ for all $i = 1, \ldots, r$ and if μ is an eigenvalue of $\mathscr{T}(D)$ with multiplicity k then -2μ is an eigenvalue of D with multiplicity $k - 1$. This follows since (7) in this case has the factor $(\lambda + 2\mu)^{k-1}$. More results concerning the characteristic polynomial of D are given in the next two theorems.

Theorem 3.2. *Let $D \neq 0$ be an $n \times n$ spherical EDM of embedding dimension r. Then the r negative eigenvalues of D are precisely the eigenvalues of $-2\mathscr{T}(D)$ if and only if the positive eigenvalue of D is equal to $e^{\mathrm{T}} De/n$.*

Proof. Suppose that the r negative eigenvalues of D are precisely the eigenvalues of $-2\mathscr{T}(D)$. Then from trace $D = 0$ and (1), it follows that the positive eigenvalue of $D = 2$ trace $\mathscr{T}(D) = e^{\mathrm{T}} De/n$.

On the other hand suppose that the positive eigenvalue of $D = e^{\mathrm{T}}De/n$. Then it follows from (7) that $b_i = 0$ for all $i = 1, \ldots, r$. Hence, the result follows. □

Following Hayden and Tarazaga [6], we say that a spherical EDM D is generated by a *regular figure* if the points that generate D lie on a hypersphere centered at the origin.[1] Recall that since $P^{\mathrm{T}}e = 0$, the centroid of the points $p^1, \ldots, p^n$ also coincides with the origin. The set of spherical EDMs generated by regular figures is characterized as the subset of EDMs having e as an eigenvector. The "only if" part of the following result was first obtained in [6].

Theorem 3.3. *Let $D \neq 0$ be an $n \times n$ spherical EDM with embedding dimension r. Then D is generated by a regular figure if and only if the r negative eigenvalues of D are precisely the eigenvalues of $-2\mathscr{T}(D)$.*

Proof. Assume that $D \neq 0$ is a spherical EDM generated by a regular figure. Then $P^{\mathrm{T}}De = 0$ since e is an eigenvector of D. Hence, $b_i = 0$ for all $i = 1, \ldots, r$. Thus, the r negative eigenvalues of D are exactly the eigenvalues of $-2\mathscr{T}(D)$.

On the other hand assume that the r negative eigenvalues of a spherical EDM D are exactly the eigenvalues of $-2\mathscr{T}(D)$. Then the positive eigenvalue of D is equal to $\frac{1}{n}e^{\mathrm{T}}De$. Hence, $b_i = 0$ for all $i = 1, \ldots, r$. Thus, $P^{\mathrm{T}}De = 0$ which implies that $De = \alpha e$ for some scalar α since $N(D) = G(D)$. Hence, the result follows. □

4. The case of non-spherical EDMs

Let D be a non-spherical EDM of embedding dimension r. Then it follows from Lemma 3.1 that $r \leqslant n - 2$ and rank $D = r + 2$. The next theorem presents a characterization of the nullspace of D.

Theorem 4.1. *Let D be a non-spherical EDM of embedding dimension r and let $\langle x \rangle$ denote the subspace generated by vector x. Then $N(D) \oplus \langle x \rangle = G(D)$, where x is the unique vector such that* $\begin{cases} Dx = e & \text{if } r = n-2, \\ Dx = e,\ x \perp N(D) & \text{if } r \leqslant n-3. \end{cases}$

Proof. Let D be a non-spherical EDM with embedding dimension r and let Z be a Gale matrix corresponding to D. Thus it follows from Lemma 2.1 and Lemma 3.1 that $DZ = [\alpha_1 e \quad \alpha_2 e \quad \cdots \quad \alpha_{\bar{r}} e] \neq 0$. If $r = n - 2$ then rank $D = n$ and $\bar{r} = 1$. Thus, $N(D)$ is trivial and Z is $n \times 1$. Hence, $\alpha_1 \neq 0$ and $x = Z/\alpha_1$. Now suppose that $r \leqslant n - 3$, i.e., $\bar{r} \geqslant 2$ then without loss of generality assume that $\alpha_1 \neq 0$. Let $y = Z_{.1}/\alpha_1$ where $Z_{.1}$ denotes the first column of Z. Then $Dy = e$. Now define the non-singular $\bar{r} \times \bar{r}$ matrix

$$Q = \begin{bmatrix} \alpha_1^{-1} & -\alpha_2 & -\alpha_3 & \cdots & -\alpha_{\bar{r}} \\ 0 & \alpha_1 & 0 & \cdots & 0 \\ 0 & 0 & \alpha_1 & \cdots & 0 \\ 0 & 0 & \ddots & \cdots & 0 \\ 0 & 0 & 0 & \cdots & \alpha_1 \end{bmatrix}.$$

[1] Some authors refer to such EDMs as EDMs of strength 1 [8,9].

Then obviously $ZQ = [y \quad \overline{Z}]$ is a Gale matrix where $\overline{Z}$ is $n \times (\bar{r} - 1)$, and $D[y \quad \overline{Z}] = [e \quad 0]$. Thus $R(\overline{Z}) \subseteq N(D)$. But rank $D = r + 2$ since D is non-spherical. Hence $\dim N(D) = \bar{r} - 1$. Therefore, $R(\overline{Z}) = N(D)$. Now let $x = (I - \overline{Z}(\overline{Z}^{\mathrm{T}}\overline{Z})^{-1}\overline{Z}^{\mathrm{T}})y$. Hence $Dx = e$ and $x^{\mathrm{T}}\overline{Z} = 0$. Thus the result follows. □

The following corollary is immediate.

Corollary 4.1. *Let D be a non-spherical EDM and let P be a realization of D. Then $R(D) = R([P \quad e \quad x])$, where x is as defined in Theorem 4.1.*

Note that for a non-spherical EDM D of embedding dimension r, $\dim N(D) = n - 2 - r = \bar{r} - 1 = \dim G(D) - 1$ and $\dim R(D) = r + 2 = \dim R([P \quad e \quad x])$. Also note that whether an EDM D is spherical or not the matrix $[P \quad e]$ is in the rangespace of D. The fact that e is in the rangespace of D was first observed by Gower in [5].

Let $Q = [P\Lambda^{-1/2} \quad e/\sqrt{n} \quad x/(x^{\mathrm{T}}x)^{1/2}]$ where P is as defined in (3). Then the non-zero eigenvalues of D are the same as the eigenvalues of $Q^{\mathrm{T}}DQ$. But

$$Q^{\mathrm{T}}DQ = \begin{bmatrix} -2\Lambda & \frac{1}{\sqrt{n}}\Lambda^{-1/2}P^{\mathrm{T}}De & 0 \\ \frac{1}{\sqrt{n}}e^{\mathrm{T}}DP\Lambda^{-1/2} & \frac{1}{n}e^{\mathrm{T}}De & \sqrt{n/x^{\mathrm{T}}x} \\ 0 & \sqrt{n/x^{\mathrm{T}}x} & 0 \end{bmatrix}. \tag{8}$$

Thus, the characteristic polynomial of an $n \times n$ non-spherical EDM D is given by

$$p(\lambda) = \lambda^{n-r-2}\left[\left(\lambda\left(\lambda - \frac{1}{n}e^{\mathrm{T}}De\right) - \frac{n}{x^{\mathrm{T}}x}\right)\prod_{i=1}^{r}(\lambda - a_i) - \lambda\sum_{i=1}^{r}b_i^2\prod_{j=1, j\neq i}^{r}(\lambda - a_j)\right], \tag{9}$$

where r is the embedding dimension of D, a_i and b_i are as defined in (7) i.e., a_i and b_i are the ith coordinates of the vectors $-2\operatorname{diag} P^{\mathrm{T}}P = -2\operatorname{diag}\Lambda$ and $\frac{1}{\sqrt{n}}(P^{\mathrm{T}}P)^{-1/2}P^{\mathrm{T}}De$ respectively, and x is as defined in Theorem 4.1.

Note that similar to the case of spherical EDMs, the coefficient of λ^{n-1} in (9) is zero. Also, if $b_{i_0} = 0$ for some i_0, $1 \leqslant i_0 \leqslant r$, then a_{i_0} is an eigenvalue of D. Furthermore, the following theorem follows easily from (9). We say that an EDM D is *centrally symmetric* if the realization matrix P corresponding to D can be written, possibly by relabeling the points p^is, as $P = \begin{bmatrix} P_1 \\ P_2 \\ P_3 \end{bmatrix}$, where $P_2 = -P_1$ and P_3 is either vacuous or the zero matrix.

Theorem 4.2. *Let D be a non-spherical centrally symmetric EDM of embedding dimension r. Then r of the negative eigenvalues of D are equal to the eigenvalues of $-2\mathscr{T}(D)$, the $r+1$th negative eigenvalue of $D = \frac{e^{\mathrm{T}}De}{2n} - \sqrt{\frac{(e^{\mathrm{T}}De)^2}{4n^2} + \frac{n}{x^{\mathrm{T}}x}}$, and the positive eigenvalue of $D = \frac{e^{\mathrm{T}}De}{2n} + \sqrt{\frac{(e^{\mathrm{T}}De)^2}{4n^2} + \frac{n}{x^{\mathrm{T}}x}}$, where x is as defined in Theorem 4.1.*

Proof. Let D be a non-spherical centrally symmetric EDM generated by points $p^1, \ldots, p^n$. Then, $P^{\mathrm{T}}De = nP^{\mathrm{T}}\operatorname{diag}\mathscr{T}(D) = n\sum_{i=1}^{n}\|p^i\|^2p^i = 0$. Hence, $b_i = 0$ for all $i = 1, \ldots, r$ and the result follows since in this case, $p(\lambda)$ reduces to $\lambda^{n-r-2}(\lambda(\lambda - \frac{1}{n}e^{\mathrm{T}}De) - \frac{n}{x^{\mathrm{T}}x})\prod_{i=1}^{r}(\lambda - a_i)$. $\square$

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