Distance Matrices and Regular Figures

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ABSTRACT

A regular figure (which includes all regular polygons) is a set of points on a hypersphere whose center coincides with their centroid. We characterize all regular figures as those whose points generate a Euclidean distance matrix (EDM) with eigenvector e, the vector of all ones. Restricting the classical maps of Schoenberg, Gower, and Critchley for all EDMs to the subcone of EDMs with eigenvector e yields new geometrical information about the generating points and a simple formula for the radius of the hypersphere.

1. INTRODUCTION

Our goal is to identify specific properties of Euclidean distance matrices (EDMs) that give special structure to the points that generate the EDM, and to study the converse relationship. We find that the set of EDMs which have e, the vector of all ones, as an eigenvector characterizes those regular figures whose points lie on a hypersphere whose center coincides with their centroid.

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Hence this class of matrices represents all regular polygons, for example. The eigenvalue λ for e has the value e^TDe/n, and the radius squared of the hypersphere is $\lambda/2n$. Furthermore (λ, e) constitute a Perron Frobenius eigenpair.

The desire to recognize special structures by properties of the distance matrix is motivated in part by our goal to predict the structure of biological molecules from information about the distances between the atoms. In many cases we know that there are special structures within the molecule, for example ring structures, helices, and beta sheets. The general problem of predicting molecular structure from incomplete data is a difficult problem; see for example [1] and [3]. Identification of regular substructures may be helpful in the solution of the general problem. Hendrickson [7] advocates a divide and conquer strategy in which one finds subsets of a structure to be minimized and then joins these substructures together for the minimization of the complete structure. In drug design, these substructures might suggest conformations that can serve as a template for the design by a pharmaceutical chemist of rigid analogues active at a specific site. Finding regular substructures from special properties of the eigenvalues and eigenvectors of a distance matrix is under current investigation.

A nonnegative symmetric $n \times n$ matrix $D = [d_{ij}^2]$ with zero on the diagonal is called a predistance matrix. If there exist n points $p_1, \dots, p_n$ in R^d such that $d_{ij}^2 = \|p_i - p_j\|^2$, then D is called a Euclidean distance matrix, and the smallest value of d is called the embedding dimension and is denoted by $E(D)$.

Gower reformulated earlier characterizations of distance matrices given by Schoenberg from the following linear algebra viewpoint [4]. Let D_1 be a predistance matrix, and suppose $G = -\frac{1}{2}D_1$. Then D_1 is a EDM if and only if

$$F = (I - es^T)G(I - se^T) \tag{1}$$

is positive semidefinite, where e is the vector of all ones and s is any vector such that $s^Te = 1$. If $F = XX^T$, so that the rows of X give the coordinates of the points that generate the distances, one observes that $X^Ts = 0$, so that s determines the position of the origin. The choices $s = e/n$ and $s = e_i$, the ith coordinate vector, place the origin at the centroid and the ith point of the configuration respectively.

Following Critchley [2], who studied the case of $s = e/n$ in detail, let

$$S_C = \{C \mid C = C^T \quad \text{and} \quad Ce = 0\} \tag{2}$$

and

$$S_H = \{H \mid H = H^T \quad \text{and} \quad H * I = 0\}, \tag{3}$$

where $H * I$ is the Hadamard product. The subspace S_C contains all centered matrices, and the subspace S_H contains all hollow matrices. The dimension of these subspaces is $n(n-1)/2$. Let $J = ee^T/n$ and define the following maps after Critchley:

$$\tau : S_H \to S_C \quad \text{and} \quad \kappa : S_C \to S_H \tag{4}$$

by

$$\tau(H) = -\tfrac{1}{2}(I-J)H(I-J), \tag{5}$$

$$\kappa(C) = (C * I)ee^T + ee^T(C * I) - 2C. \tag{6}$$

Critchley establishes many properties of these maps, including the following result.

THEOREM 1.1. *The mappings κ and τ are linear and mutually inverse.*

2. REGULAR FIGURES

We now examine the mappings κ and τ on some special subsets of S_C and S_H where the mappings have a very simple form. Let

$$\Omega_n(e) = \{A \in \Omega_n \mid Ae = 0 \text{ and } a_{ii} = a \text{ for } i = 1, 2, \ldots, n\},$$

and

$$\Lambda_n(e) = \{D \in \Lambda_n \mid De = \lambda e\}$$

be subsets of the cone of positive semidefinite matrices and the cone of EDMs respectively. Note that they are also convex cones. For $A \in \Omega_n(e)$ the coordinates of $\kappa(A)$ are given by the rows of C if $A = CC^T$. From the definition of $\Omega_n(e)$, C must satisfy $C^Te = 0$, and the two-norm of every row is constant. The first condition implies that the centroid of the points is at the origin, and the second condition says each point lies on a sphere with center at the origin.

The following results are straightforward application of the definitions, and hence only brief outlines of the proofs are included.

LEMMA 2.1. *Given $A \in \Omega_n(e)$ and $D \in \Lambda_n(e)$, then*

$$\kappa(A) = 2aee^T - 2A \tag{7}$$

and

$$\tau(D) = -\frac{1}{2}D + \frac{e^TDe}{2n^2}ee^T. \tag{8}$$

Note that e^TDe/n is the eigenvalue that corresponds to the eigenvector e.

To prove (8) note that $I - J$ is a projection that commutes with D, since e is an eigenvector of D. We show in the next section that distance matrices have only one positive eigenvalue, and hence a computation yields the following corollary.

COROLLARY 2.1. *If $D \in \Lambda_n(e)$, then $\left(\frac{e^TDe}{e^Te}, e\right)$ is a Perron-Frobenius eigenpair.*

LEMMA 2.2. *One has*

$$\kappa(\Omega_n(e)) = \Lambda_n(e),$$

$$\tau(\Lambda_n(e)) = \Omega_n(e).$$

Furthermore,

$$\|\kappa(A)\|^2 = 4\left[\|A\|^2 + (na)^2\right],$$

$$\|\tau(D)\|^2 = \frac{1}{4}\left[\|D\|^2 - \left(\frac{e^TDe}{e^Te}\right)^2\right].$$

The norm is the Frobenius matrix norm.

COROLLARY 2.2. *Given $D \in \Lambda_n(e)$, all diagonal elements of $\tau(D)$ are equal to*

$$\frac{e^TDe}{2n^2},$$

and all the points of the configuration lie on a sphere with radius R, *where*

$$R^2 = \frac{e^T De}{2n^2} \tag{9}$$

The proof is a consequence of (8) and the fact that $\tau(D) = CC^T$.

The set

$$M = \{x \in R^n \mid x^T e = 0\} \tag{10}$$

is fundamental, since a distance matrix is a EDM if and only if the distance matrix is positive semidefinite on M. In [6] we obtained the following representation. If $D \in \Lambda_n$ then there exists $v_i \in M$, $i = 1, \dots, r$, $z \in M$, where $r = E(D)$, such that

$$-\frac{1}{2}D = \sum_{i=1}^{r} v_i v_i^T + ze^T + ez^T + \alpha ee^T. \tag{11}$$

Furthermore we showed that D has rank $r + 1$ if and only if z is in the span of $v_1, \dots, v_r$. We are able to characterize $\Lambda_n(e)$ from this formula.

THEOREM 2.1. *Suppose* $D \in \Lambda_n$ *and* $D \neq 0$. *Then* $D \in \Lambda_n(e)$ *if and only if* $z = 0$ *in the representation* (11). *Furthermore if* $D \in \Lambda_n(e)$ *and* $E(D)$ *is* r, *then* rank $D = r + 1$.

A geometrical characterization of our subcone $\Lambda_n(e)$ can be obtained by the following observations. $\tau(D)e = 0$ if and only if the centroid is the origin of the coordinates. Also, $\tau(D)_{ii}$ is constant if and only if the points generating D lie on the surface of a sphere with center the origin.

THEOREM 2.2. *If* $D \in \Lambda_n$, *then the following statements are equivalent*:

(i) $D \in \Lambda_n(e)$

(ii) *The points which generate* D *lie on the surface of a sphere whose center is the centroid of the points.*

Proof. By Lemma 2.2, $D \in \Lambda_n(e)$ if and only if $\tau(D) \in \Omega_n(e)$. Because of the comment after the definition of $\Omega_n(e)$, $\tau(D) \in \Omega_n(e)$ if and only if (ii) holds. ■

3. EIGENVALUE RELATIONS AND RADIUS FORMULA

For $D \in \Lambda_n(e)$ we observed that

$$R^2 = \frac{e^T De}{2n^2}.$$

The following theorem generalizes the above formula to the case where the center of the hypersphere containing the generating points and the centroid may differ.

THEOREM 3.1. *Suppose the points which generate the EDM D lie on the surface of a sphere with center zero and radius R, and have centroid c. Then*

$$R^2 = \|c\|^2 + \frac{e^T De}{2n^2}. \tag{12}$$

Proof. Let $x_1, x_2, \dots, x_n$ denote the points which generate the EDM D and lie on the surface of a sphere with center zero and radius R. Suppose $E(D) = r$ and let X be the n by r matrix with x_i^T the ith row of X. Applying elementary relationships between the points and the distances they generate, one can easily show that

$$-\frac{D}{2} = XX^T - \bar{x}e^T - e\bar{x}^T, \tag{13}$$

where

$$\bar{x} = \tfrac{1}{2}\left(x_1^T x_1, x_2^T x_2, \dots, x_n^T x_n\right)^T.$$

Note that Equation (13) holds for all configurations of points, not just the special case under consideration. Now in case the points lie on a hypersphere with center zero and radius R, then

$$\bar{x} = \tfrac{1}{2}R^2 e,$$

$$-\tfrac{1}{2}D = XX^T - R^2 ee^T.$$

Hence

$$-\tfrac{1}{2}e^TDe = e^TXX^Te - R^2n^2 = n^2\left(\left\|\frac{X^Te}{n}\right\|^2 - R^2\right). \qquad \square$$

We next consider the relationship between the spectrum of the EDM D and the spectrum of the positive semidefinite matrix $\tau(D)$. The case where $D \in \Lambda(e)$ is particularly simple.

THEOREM 3.2. *Suppose $D \in \Lambda_n(e)$, $D \neq 0$, and $-D$ has r positive eigenvalues. Then $-D$ has one negative eigenvalue. $\tau(D)$ has the same r positive eigenvalues as $-D/2$, and $n - r$ zero eigenvalues. Hence* rank $(D) = r + 1$ *and* rank $(\tau(D)) = r$.

Proof. We will show in the next theorem that $-D$ has exactly one negative eigenvalue for all EDMs. Since $De = \lambda e$, one can show $DJ = JD = \lambda J$. For $D \in \Lambda_n(e)$ we have $\tau(D) = \frac{1}{2}(\lambda J - D)$. The rank one matrix λJ has $\lambda Je = \lambda e$ and all other eigenvalues zero. Since J and D commute, they are simultaneously diagonalizable. Hence using the spectral decomposition, we have

$$\lambda J - D = \lambda\frac{ee^T}{n} - \left(\lambda\frac{ee^T}{n} + \cdots + \lambda_n u_n u_n^T\right).$$

Therefore $\tau(D)$ has the same eigenvalues as $-D/2$ with the negative eigenvalue of $-D$ set to zero. The other statements follow from the definitions. ■

The next result extends the eigenvalue comparison of D and $\tau(D)$ to all EDMs.

THEOREM 3.3. *If $D \neq 0$ is a EDM, then $-D$ has one negative eigenvalue. Let r be the rank of the positive semidefinite matrix $\tau(D)$. Then $-D$ has either r or $r+1$ positive eigenvalues, so* rank *D is $r+1$ or $r+2$. The positive eigenvalues of $-D/2$ are interlaced by the positive eigenvalues of $\tau(D)$.*

Proof. By a result of Hayden and Wells [5], D is a EDM if and only if

$$Q(-D)Q = \begin{pmatrix} -\overline{D} & d \\ d^T & \delta \end{pmatrix},$$

where $-\overline{D}$ is positive semidefinite and $Q = I - 2vv^T/v^Tv$ for $v = [1, 1, 1, \ldots, 1 + n^{1/2}]^T$. The embedding dimension is $r = \text{rank}(-\overline{D})$. Since

$$Q(I - J)Q = \begin{pmatrix} I_{n-1} & 0 \\ 0 & 0 \end{pmatrix},$$

then

$$2\tau(D) = Q\begin{pmatrix} -\overline{D} & 0 \\ 0 & 0 \end{pmatrix}Q.$$

Since $-\overline{D}$ has r positive eigenvalues and $n - 1 - r$ zero eigenvalues, then $\tau(D)$ has the same r positive eigenvalues as $-\overline{D}$ and $n - r$ zero eigenvalues, noting that Q is orthogonal. Furthermore the eigenvalues of $-\overline{D}$ interlace those of

$$Q(-D)Q = \begin{pmatrix} -\overline{D} & d \\ d^T & \delta \end{pmatrix}.$$

Since Q is orthogonal, the eigenvalues of $Q(-D)Q$ are the same as those of $-D$. Now trace$[Q(-D)Q]$ = trace$(-D) = 0$. Therefore one and only one eigenvalue of $Q(-D)Q$ is negative, using the interlacing property. Furthermore, by interlacing, the positive eigenvalues of $-\overline{D}$ interlace those of $Q(-D)Q$ and hence those of $-D$. Since the eigenvalues of $-\overline{D}/2$ are those of $\tau(D)$, the theorem is proved. ■

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