Block Matrices and Multispherical Structure of Distance Matrices

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ABSTRACT

The block structure of a matrix and its relation to the block structure of the corresponding eigenvectors is investigated. A set of points is said to have multispherical structure if they lie on a collection of concentric spheres. When the centroid of each of the clusters lies at the common center, the associated distance matrix has a block structure with simple relations between the blocks. Further, such block structure may be recognized from the structure of the eigenvectors of the distance matrix. A computational procedure is proposed to find the least number of concentric spheres containing the points represented by a distance matrix.

1. INTRODUCTION

How is the structure of a Euclidean distance matrix (EDM) $D$ related to the geometrical properties of the points that generate it? Understanding this relationship should aid in drug design, in which one searches for ligands that may be competitive inhibitors of an enzyme. In some cases the geometry of the binding site is known, and in other cases one may try to

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predict the geometry of the binding site by observing the binding constants for different orientations of several small ligands. The geometry is only one facet of this difficult problem, in which energetics and many other factors play a role.

Since the force field is often spherical and spheres are a simple first approximation to binding sites, we investigate the connection between the EDM and the geometry of the points that generate it for the simple case involving a cluster of points, each lying on some sphere. We find that spherical geometry among the generating points induces block structure in the associated distance matrix and that block structure of the EDM plus other conditions yields spherical geometry.

In [5] we found that the points that generate an EDM $D$ lie on a sphere with common centroid and center if and only if the row sums are constant, or equivalently the vector $e$ of all ones is an eigenvector of $D$. This result was generalized in [7] for the case in which the points lie on a sphere whose center and centroid no longer coincide. In this case the corresponding condition is that the weighted row sums are constant or, more precisely, there exists a vector $s$ with $s^Te = 1$ such that $Ds = \beta e$ for some real $\beta$. In this paper we extend these results by showing that if the distance matrix can be blocked so that the blocks have constant row sums, then the points generating the EDM lie on multiple spheres all having common centers and centroids. By considering blocks with constant weighted row sums and some additional conditions we can extend to the case where the centers and centroids no longer coincide. We also establish that block eigenvectors of the EDM are related to these multispherical structures.

We begin, in Section 3, with an investigation of the block structure of general symmetric matrices and show that the existence of matrix block structure is equivalent to the existence of block structure of certain of its eigenvectors. Next, in Section 4, we apply these results to EDMs, particularly to the case in which the convex hull of each cluster contains the common center. A formula relating the distances between the various centroids and radii of spherical clusters in terms of the average value of the corresponding blocks is given. Section 5 presents an algorithm using mixed-integer linear programming to determine the minimal number of concentric spheres needed to contain a set of points that generate an EDM.

2. DEFINITIONS AND PRELIMINARY RESULTS

A symmetric $n \times n$ matrix $D = [d_{ij}^2]$ is called a Euclidean distance matrix (EDM) if there exist points $P_1, P_2, \ldots, P_n$ in $\mathbb{R}^r (r < n)$ such that

$$d_{ij}^2 = \|P_i - P_j\|^2 \quad (i \leq i, j \leq n).$$

(1)
The smallest such \( r \) is called the *embedding dimension* of \( D \). Of course, for every such \( r \) there are many such representing configurations, any two being related by a linear isometry. For example, given an EDM \( D \), one may search for a representation such that \( P_1 + \ldots + P_n = 0 \), or such that \( P_i = 0 \) for a particular choice of \( i \). To provide a systematic approach, we choose a vector \( s \in \mathbb{R}^n \) such that \( s^T e = 1 \), with \( e = [1, 1, \ldots, 1]^T \in \mathbb{R}^n \), and based on any such choice for \( s \), we define

\[
B = -\frac{1}{2}(I - es^T)D(I - se^T). \tag{2}
\]

Clearly \( Bs = 0 \). Furthermore, \( B \) is positive semidefinite and accordingly can be factored in the form \( B = XX^T \). If \( P_1^T, \ldots, P_n^T \) represents a top-to-bottom labeling of the rows of \( X \), then \( B = [P_1^T P_2^T] \) and, since \( Bs = 0 \),

\[
s_1P_1 + s_2P_2 + \cdots + s_nP_n = 0. \tag{3}
\]

Let \( e_i = (0, 0, \ldots, 1, 0, \ldots, 0)^T \) be the \( i \)th standard unit vector. The calculation \((e_i^T - e_j^T)(B + \frac{1}{2}D)(e_i - e_j) = 0\) shows that the relations (1) hold; hence \( P_1, \ldots, P_n \) is a representing configuration for \( D \). Moreover, if \( b \) denotes the diagonal of \( B \), then

\[
b = [\|P_1\|^2, \ldots, \|P_n\|^2]^T, \tag{4}\]

and \( D \) is recovered from \( B \) via the formula

\[
D = be^T + eb^T - 2B. \tag{5}\]

For obvious reasons, we call \( B \) a *coordinate matrix* for \( D \), and say that the vector \( s \) *fixes* the coordinate system. This and related ideas are introduced and developed in [3], [4], and [1].

In general, the evidence for an EDM \( D \) being represented by a spherical or a multispherical structure may be found by examining certain weighted row sums or weighted row sums within blocks. The first result in this direction is that \( D \) is represented by a single spherical structure with its center and centroid at the origin if and only if \( e \) is an eigenvector of \( D \); thus, if and only if the row sums are constant [5]. Second, \( D \) is represented by a single spherical structure centered at the origin if and only if \( Ds = \beta e \) for some vector \( s \), \( s^T e = 1 \) [7].

Given an EDM \( D \) and a coordinate choice \( s \), we understand a basic multispherical structure of \( D \) to be the following information:

(a) the number of spheres centered at the origin necessary to contain a representing set of points for \( D \), and

(b) the number of points on each sphere.
Lemma 2.1. Suppose \( s \in \mathbb{R}^n \), \( s^T e = 1 \), and \( D \) is an EDM. Then the components of \( Ds \) identify the basic multispherical structure of a set of generating points for \( D \) relative to the coordinate system fixed by the choice of \( s \).

Proof. If we compute \( B \) from \( D \) via (2), then (5) holds and

\[
Ds = b + (b^T s)e.
\] (6)

Therefore \( Ds \) is the sum of \( b \) and a constant vector. Now since the vector \( b \) gives the squares of the distances of a set of representing points from the origin, it follows that the basic spherical structure of \( D \) is reflected in \( Ds \). In other words, the number of distinct values in the range of \( Ds \) determines the number of spheres, and the number of preimages for each such value determines the number of points in that sphere.

A vector \( x \in \mathbb{R}^n \) is said to have block structure if it can be partitioned into \( k \) blocks \((k < n)\) so that \( x \) has a constant value in each block. Of course, the vector \( Ds \) of the preceding lemma need not be blocked. But there will always exist a permutation \( P \) such that \( PDs \) is a block vector and the EDM \( PDP^T \) will have the same multispherical structure as \( D \). In the rest of the paper we will always assume that such a permutation has been applied.

3. Block Structure

Throughout this section \( n_1, n_2, \ldots, n_k \) denote positive integers such that \( n_1 + n_2 + \cdots + n_k = n \,(n < k) \), \( \sigma_i \) denotes the vector of all ones in \( \mathbb{R}^{n_i} \), and, when convenient, an \( n \times n \) matrix \( D \) will be considered as a \( k \times k \) matrix of blocks \( D_{ij} \) having dimensions \( n_i \times n_j \). To facilitate the labeling process we put

\[
q_0 = 0, \quad q_1 = n_1, \quad q_2 = n_1 + n_2, \quad \ldots, q_k = n_1 + \cdots + n_k = n.
\]

With the partition \( n_1, \ldots, n_k \) we associate a sequence of weights \( s_j \in \mathbb{R}^{n_j} \) such that

\[
s_j^T \sigma_j = n_j \quad (j = 1, \ldots, k).
\] (7)

Let

\[
S = \text{diag}[s_1^T, s_2^T, \ldots, s_k^T].
\]

Then, if the \( n \times n \) matrix \( D \) is blocked according to the partition \( n_1, \ldots, n_k \), the product \( DS \) places the weights of \( s_j \) appropriately with the elements of each row in the block \( D_{ij} \).
Although we intend to apply the results of this section to EDMs, all results for block structure are valid for an arbitrary symmetric matrix.

**DEFINITION 3.1.** A symmetric $n \times n$ matrix $D$ has $s$-block structure if there exists a $k \times k$ matrix $A = [a_{ij}]$ such that

$$D_{ij}s_j - a_{ij} = (i, j = 1, \ldots, k).$$  \hspace{1cm} (8)

Since $D$ is symmetric, an examination of $s_i^T D_{ij}s_j$ and $s_j^T D_{ji}s_i$ in (8) shows that

$$n_i a_{ij} = n_j a_{ji} \quad (i, j = 1, \ldots, k).$$  \hspace{1cm} (9)

Thus, although the matrix $A$ need not be symmetric, it is similar to the symmetric matrix

$$N^{1/2} A N^{-1/2} = [n_i^{1/2} a_{ij} n_j^{-1/2}], \quad N = \text{diag}[n_1, n_2, \ldots, n_k]^T$$

and therefore has a complete set of eigenvectors.

**THEOREM 3.1.** A symmetric $n \times n$ matrix $D$ has $s$-block structure if and only if the matrix $DS$ has $k$ linearly independent block eigenvectors.

**Proof.** If $D$ has $s$-block structure, then, using the notation introduced above, the matrix $A$ has $k$ linearly independent eigenvectors $v_1, v_2, \ldots, v_k$ in $R^k$; hence

$$Av_j = \lambda_j v_j, \quad j = 1, \ldots, k.$$  \hspace{1cm} (10)

We define block vectors $\tilde{v}_1, \tilde{v}_2, \ldots, \tilde{v}_k$ in $R^n$ by

$$\tilde{v}_j = [v_{j1} \sigma_1^T, \ldots, v_{jk} \sigma_k^T]^T.$$  \hspace{1cm} (11)

Then, for $p = 1, \ldots, k$,

$$DS\tilde{v}_p = \left[ \left( \sum_{j=1}^{k} v_{pj} D_{1js_j} \right)^T, \left( \sum_{j=1}^{k} v_{pj} D_{2js_j} \right)^T, \ldots, \left( \sum_{j=1}^{k} v_{pj} D_{kjs_j} \right)^T \right]^T$$

$$= \left[ \sum_{j=1}^{k} v_{pj} a_{1j} \sigma_1^T, \sum_{j=1}^{k} v_{pj} a_{2j} \sigma_2^T, \ldots, \sum_{j=1}^{k} v_{pj} a_{kj} \sigma_k^T \right]^T$$

$$= \left[ \lambda_p v_{p1} \sigma_1^T, \lambda_p v_{p2} \sigma_2^T, \ldots, \lambda_p v_{pk} \sigma_k^T \right]^T$$

$$= \lambda_p \tilde{v}_p.$$
Conversely, suppose there are \( k \) linearly independent block eigenvectors of \( DS \) given by (11). In order to show that \( D \) has \( s \)-block structure, we focus on systems of equations that arise by considering particular components, one from each of the equations

\[
DS\vec{v}_j = \lambda_j\vec{v}_j \quad (j = 1, \ldots, k).
\]  

(12)

In the matrix \( DS \) consider the block sums defined by

\[
S_{i1} = \sum_{j=1}^{q_1} d_{ij} s_{1j}, \quad i = 1, \ldots, n,
\]

\[
S_{i2} = \sum_{j=1}^{n_2} d_{i,j+q_1} s_{2j}, \quad i = 1, \ldots, n,
\]

\[
S_{ik} = \sum_{j=1}^{n_k} d_{i,j+q_{k-1}} s_{kj}, \quad i = 1, \ldots, n.
\]  

(13)

Using this notation, the system of first components from each of the \( k \) vector equations in (12) is

\[
v_{11}S_{11} + v_{12}S_{12} + \cdots + v_{1k}S_{1k} = \lambda_1v_{11},
\]

\[
v_{21}S_{11} + v_{22}S_{12} + \cdots + v_{2k}S_{1k} = \lambda_2v_{22},
\]

\[
\vdots
\]

\[
v_{k1}S_{11} + v_{k2}S_{12} + \cdots + v_{kk}S_{1k} = \lambda_kv_{k1}.
\]  

(14)

Since the vectors \( \vec{v}_1, \ldots, \vec{v}_k \) are linearly independent,

\[
\begin{bmatrix}
S_{11} \\
S_{12} \\
\vdots \\
S_{1k}
\end{bmatrix} = \begin{bmatrix}
v_{11} & v_{12} & \cdots & v_{1k} \\
v_{21} & v_{22} & \cdots & v_{2k} \\
\vdots & \vdots & \ddots & \vdots \\
v_{k1} & v_{k2} & \cdots & v_{kk}
\end{bmatrix}^{-1} \begin{bmatrix}
\lambda_1v_{11} \\
\vdots \\
\lambda_kv_{k1}
\end{bmatrix}.
\]  

(15)

Supposing that \( n_1 > 1 \), we look next at the system of second components from (12). Clearly, the only change in (15) is that \( S_{1j} \) is replaced by \( S_{2j} \). Hence, \( S_{1j} = S_{2j} \), \( j = 1, 2, \ldots, k \). That is, within the first row of blocks of widths \( n_1, n_2, \ldots, n_k \), respectively, the first two rows have the same weighted averages. The same situation holds through the first \( n_1 \) rows. At row \( n_1 + 1 \), the right side in (15) changes but remains fixed for rows with indices \( n_1 + 1 \) to \( n_1 + n_2 \). Therefore, \( D \) has \( s \)-block structure.
We will make special use of the case \( s_j = \sigma_j \). Here, (8) becomes the assumption that the row sums are constant within each block \( D_{ij} \), and the assertion in Theorem 3.1 is that \( D \) has \( k \) block eigenvectors. Further, we observe that the existence of block eigenvectors provides useful information concerning the remaining eigenvectors.

**Theorem 3.2.** Suppose \( D = D^T \) has \( k \)-block structure with constant row sums within each block, and \( \tilde{v}_1, \ldots, \tilde{v}_k \) are \( k \) linearly independent eigenvectors of \( D \) with the corresponding block structure. If \( w \) is an eigenvector of \( D \) that is orthogonal to each of \( \tilde{v}_1, \ldots, \tilde{v}_k \), then each of the corresponding blocks in \( w \) has sum 0. Furthermore, if \( D \) has positive elements, the Perron-Frobenius eigenvector of \( D \) is one of the block eigenvectors.

**Proof.** Let \( w_1, \ldots, w_k \) be the sums of the corresponding blocks of the vector \( w \). Then

\[
    w^T \tilde{v}_j = w_1 v_{j1} + w_2 v_{j2} + \cdots + v_k v_{jk} = 0, \quad j = 1, \ldots, k.
\]

The conclusion \( w_j = 0, \ j = 1, \ldots, k \), now follows from the linear independence of the vectors

\[
    [v_{j1}, v_{j2}, \ldots, v_{jk}]^T, \quad j = 1, \ldots, k.
\]

The final conclusion comes from the observation that the Perron-Frobenius eigenvector has nonnegative elements and belongs to a positive eigenvalue.

**4. MULTISPERICAL STRUCTURES**

**Theorem 4.1.** Let \( D \) be an EDM. The following are equivalent:

(a) There exists a vector \( s \) such that \( s^T e = 1 \) and \( Ds \) has block structure, that is,

\[
    Ds = [v_1, \ldots, v_1, v_2, \ldots, v_2, \ldots, v_k, \ldots, v_k]^T,
\]

the blocks having lengths \( n_1, \ldots, n_k \), respectively, and \( n_1 + \cdots + n_k = n \ (k < n) \)

(b) There exist \( n \) generating points \( P_1, \ldots, P_n \) for \( D \) that lie on \( k \) spheres \( S_1, \ldots, S_k \) each centered at the origin. The sphere \( S_1 \) has radius \( R_1 \) and contains \( P_1, \ldots, P_{n_1} \); \( S_2 \) has radius \( R_2 \) and contains \( P_{n_1+1}, \ldots, P_{n_1+n_2} \), etc.
Proof. The proof that (a) implies (b) is the content of Lemma 2.1.

For the converse, we start with the points $P_1, \ldots, P_n$, define $b$ as in (4), let $B = [P_i^T P_j]$, and express $D$ in terms of $b$ and $B$ via (5). Note that $b$ has block structure. If there exists a vector $s$, with $s^T e = 1$, such that $Bs = 0$, then $Ds$, given by (5), has block structure also.

If no such $s$ exists, then $Bs = 0$ only holds when $s^T e = 0$, so that $N(B) \subset M = \{x : x^T e = 0\}$. Hence $Rg(B) \supset M^\perp = \langle e \rangle$. Consequently, there exists a vector $s$ such that $Bs = e$, and from $s^T Bs = s^T e$ we conclude that $s^T e \neq 0$. Using this $s$ (that $s^T e$ may not be 1 is unimportant), we find that

$$Ds = b(e^T s) + e(b^T s) - 2e.$$  

Again, the block structure of $b$ is passed on to $Ds$. Hence (b) implies (a).

This theorem places no restriction on the locations of the centroids of the various spherical clusters. In the next theorem, additional conditions are imposed on $D$ to force each cluster to have the origin in its convex hull.

**Theorem 4.2.** Let $D$ be an EDM blocked so the $D_{ij} \in R^{n_i \times n_j}$, and suppose that the weight sequences $s_1, \ldots, s_k$ are nonnegative. The following are equivalent:

(a) There exists a $k \times k$ matrix $A = [a_{ij}]$ such that

$$D_{ij} s_j = a_{ij} \sigma_i$$

and

$$\frac{a_{ij}}{n_j} = \frac{a_{ji}}{n_i} = \frac{a_{ii}}{2n_i} + \frac{a_{jj}}{2n_j}$$

for $i, j = 1, \ldots, k$.

(b) There exist $n$ generating points $P_1, P_2, \ldots, P_n$ for $D$ that lie in $k$ spheres $S_1, S_2, \ldots, S_k$, each centered at the origin $0$. The sphere $S_1$ contains $P_1, \ldots, P_n$; $S_2$ contains $P_{n+1}, \ldots, P_{n+n_2}$, etc., and each of the separate spherical configurations has the origin in its convex hull.

(c) The matrix $DS$ has $k$ block eigenvectors that belong to the null space of $BS$ (recall $S = \text{diag}(s)$).

Proof. As we observed earlier in (9), the relations

$$n_i a_{ij} = n_j a_{ji}$$


follow from (16). Hence the first equality in (17) is a consequence of (16). Adding the equalities in (17) gives the relations

\[ \sum_{j=1}^{k} a_{ij} = \frac{n}{2n_i} a_{ii} + \frac{1}{2} \sum_{j=1}^{k} a_{jj}, \quad i = 1, \ldots, k, \]

which relate \( \text{tr}(A) \) to its row sums.

To prove that (a) implies (b), we use the weight vectors to define

\[ \tilde{s} = \frac{1}{n} [s_1^T, s_2^T, \ldots, s_k^T]^T = [\tilde{s}_1^T, \tilde{s}_2^T, \ldots, \tilde{s}_n^T]^T. \]

Then \( \tilde{s}^T e = 1 \), and the coordinate matrix

\[ B = -\frac{1}{2} (I - e\tilde{s}^T) D (I - \tilde{s} e^T) \]
satisfies \( B\tilde{s} = 0 \), meaning that \( D \) is generated by points \( P_1, P_2, \ldots, P_n \) such that

\[ \tilde{s}_1 P_1 + \tilde{s}_2 P_2 + \cdots + \tilde{s}_n P_n = 0. \]

Further, \( D \) is recovered from \( B \) by

\[ D = b e^T + e b^T - 2B, \]

where \( b = [\|P_1\|^2, \ldots, \|P_n\|^2]^T \). From (16) it follows that \( D\tilde{s} \) is a block vector, and from

\[ D\tilde{s} = b(e^T \tilde{s}) + e(b^T \tilde{s}) \]

that \( b \) is a block vector; hence

\[ b = [R_1^2, \ldots, R_1^2, R_2^2, \ldots, R_2^2, \ldots, R_k^2, \ldots, R_k^2]^T. \]

Consequently, the generating points \( P_1, \ldots, P_{q_1} \) lie on a sphere of radius \( R_1 \), the points \( P_{q_1+1}, \ldots, P_{q_2} \) lie on a sphere of radius \( R_2 \), etc., all centered at the origin. Further, \( be^T, e b^T \), and \( B \) have the same block structure as \( D \), the various blocks being related by

\[ D_{ij} = R_i^2 \sigma_i \sigma_j^T + R_j^2 \sigma_i \sigma_j^T - 2B_{ij} \quad (i, j = 1, \ldots, k) \]

and, in particular

\[ D_{ii} = 2R_i^2 \sigma_i \sigma_i^T - 2B_{ii} \quad (i = 1, \ldots, k). \]
We will show that the points $P_{q_{i-1}+1}, \ldots, P_{q_i}$ that generate the diagonal block $D_{ii}$ have the origin in their convex hull by establishing that

$$s_{i1}P_{q_{i-1}+1} + \cdots + s_{in_i}P_{q_i} = 0,$$

that is, $B_{ii}s_i = 0$. From (16) and (20), this is equivalent to showing that

$$R_i^2 = \frac{a_{ii}}{2n_i}, \quad i = 1, \ldots, k.$$  \hfill (21)

To this end, recall that $B\tilde{s} = 0$. Hence $D\tilde{s} = e(b^T\tilde{s}) + b(e^T\tilde{s})$. If we equate components, use the structure for $b$, and finally multiply by $n$, we obtain

$$nR_i^2 + n_1R_1^2 + \cdots + n_kR_k^2 = \sum_{j=1}^{k} a_{ij} \quad (i = 1, \ldots, k).$$  \hfill (22)

The coefficient matrix of this system is nonsingular (its determinant is $2n^k$), and the unique solution is given by the values $R_1^2, \ldots, R_k^2$ in (21), because their substitution in (22) yields the equations (18), which hold by hypothesis. Thus (a) implies (b).

To see that (b) implies (a), suppose that $D$ is generated by points as described in (b). Define $b$ by (4) where $R_i = ||P_j||$, $j = q_{i-1} + 1, \ldots, q_i$, and $i = 1, \ldots, k$, and define $B = [P_iP_j^T]$. Then $D, b,$ and $B$ are related by (5), and the block equations (19) hold. By assumption there exist nonnegative weights $s_1, s_2, \ldots, s_k$ such that

$$\sum_{j=q_{i-1}+1}^{q_i} s_{ij}P_j = 0 \quad (i = 1, \ldots, k),$$

and therefore the $n_i \times n_j$ blocks $B_{ij}$ of $B$ satisfy

$$B_{ij}s_j = 0.$$  \hfill (23)

At this point we scale the weights $s_i$ so that $s_i^T\sigma_i = n_i$, $i = 1, \ldots, k$. In (19) this information implies

$$D_{ij}s_j = R_i^2n_j\sigma_i + R_j^2n_j\sigma_i.$$  

Hence $D_{ij}s_j = a_{ij}\sigma_i$ where

$$a_{ij} = n_j(R_i^2 + R_j^2) \quad (i, j = 1, \ldots, k)$$  \hfill (24)

and, if $i = j$,

$$R_i^2 = \frac{a_{ii}}{2n_i}.$$  \hfill (25)

Combining these last two equations, we obtain (17).
Finally, we show that (b) and (c) are equivalent. Under the assumptions in (b), $D$ has $s$-block structure and, according to Theorem 3.1, $DS$ has $k$ linearly independent block eigenvectors that are linear combinations of $[\sigma_i^T, 0, \ldots, 0]^T, \ldots, [0, \ldots, 0, \sigma_i^T]^T$. Knowing that each point cluster has the origin in its convex hull implies that $B_{ij}s_j = 0$, which, in turn, forces $BS\sigma_j = 0$, $j = 1, \ldots, k$, so that the block eigenvectors of $DS$ are in the null space of $BS$.

In the other direction, the assertion that $DS$ has $k$ linearly independent block eigenvectors implies, by Theorem 3.1, that $D$ has $s$-block structure and hence that $b$ has block structure. This latter fact forces $P_1, \ldots, P_{q_1}$ to lie on a sphere of radius $R_1$, the points $P_{q_1+1}, \ldots, P_{q_2}$ to lie on a sphere of radius $R_2$, etc. And the assumption that these block eigenvectors are in the null space of $BS$, again by Theorem 3.1 [with all the $\lambda$'s equal to 0 in (15)], implies that $B$ has $s$-block structure in which each block has weighted row sums 0. This implies that each spherical group of the $P$'s contains the origin in its convex hull.

For applications in chemistry and drug design, one might be interested in a relationship where one cluster of atoms in a specific site can be approximated by atoms on a sphere and a nearby cluster by a similar arrangement. What are the relationships between such clusters? The referee pointed out that the following result was similar to those obtained in [2]; and hence we only state the result for completeness regarding spherical structures.

Let the average of the distances in a block $D_{ij}$ of size $n_1 \times n_2$ be denoted by $\text{Ave}(D_{ij})$. If $\sigma_i$ denotes the vector of ones of length $n_i$, then $\text{Ave}(D_{ij}) = \sigma_i^T D_{ij} \sigma_j / n_i n_j$. We suppose that $n_1$ points lie on a sphere of radius $R_1$ and have centroid $c_1$, and use similar notation for a second cluster of $n_2$ points. The following theorem easily extends to $k$ clusters.

**Theorem 4.3.** Suppose $n_1 + n_2 = n$ points are on two spherical clusters with respective centroids $c_1$, radii $R_i$, and distances from the center of the sphere to the centroids denoted by $\|\hat{c}_i\|$ for $i = 1, 2$. Then

$$\frac{1}{2} \text{Ave}(D_{ii}) = R_i^2 - \|\hat{c}_i\|^2 \quad \text{for} \quad i = 1, 2,$$

$$\text{Ave}(D_{12}) = \frac{1}{2} \text{Ave}(D_{11}) + \frac{1}{2} \text{Ave}(D_{22}) + \|c_1 - c_2\|^2.$$

5. **COMPUTING THE MINIMAL NUMBER OF SPHERES**

Next, we describe a method for determining the minimum number $k^*$ of concentric spheres that contain a set of generating points for an EDM $D$. Our method relies on the technique of mixed-integer linear-programming [6]. We note that it suffices to describe a method for determining, for a given $k$
(1 \leq k \leq n), if there is a set of k concentric spheres containing a set of points that generate D. This is sufficient because we can perform a bisection search, considering integers k in the interval \([1, n]\), requiring at most \(O(\log_2 n)\) steps to find the minimizing value \(k^*\).

Recall that there are k concentric spheres containing the points when there is an n-vector \(s\) satisfying \(e^T s = 1\), with the property that \(w = Ds\) has at most \(k\) distinct coordinates. We define real variables \(v_j\) (1 \leq j \leq k) to represent the potential coordinate values. We assume that they are ordered as \(v_1 \leq v_2 \leq \cdots \leq v_k\). Next, we define binary variables \(y_{ij}\) which indicate the assignment of coordinates of the n-vector \(w\) to the k-vector \(v\). Specifically, the interpretation of \(y_{ij} = 1\) is that \(w_i\) is forced to equal \(v_j\). Let \(M\) be a sufficiently large positive constant. We can now recast the question of whether there is a set of k concentric spheres containing the points as the question of whether the following mixed-integer linear program has a feasible solution:

\[
Ds = w, \quad e^T s = 1, \quad \sum_{j=1}^{k} y_{ij} = 1 \quad (1 \leq i \leq n),
\]

\[
v_j - My_{ij} \leq w_i \leq v_j + My_{ij} \quad (1 \leq i \leq n, \quad 1 \leq j \leq k), \quad n_1 \leq v_2 \leq \cdots \leq v_k, \quad w, s \in \mathbb{R}^n, \quad v \in \mathbb{R}^k, \quad y_{ij} \in \{0, 1\} \quad (1 \leq i \leq n, \quad 1 \leq j \leq k).
\]

Conceptually, there is no added difficulty in minimizing a linear objective function over the above constraint set. One possibility is to minimize \(v_k - v_1\). For this choice of objective function, we observe that for the choice of \(k = 2\), the solution reveals whether one or two or more than two spheres are necessary.

The linear relaxation of the mixed-integer linear program is the program obtained by replacing the restrictions \(y_{ij} \in \{0, 1\}\) with \(0 \leq y_{ij} \leq 1\). The behavior of any method to solve a mixed-integer linear program is related to the degree to which the linear relaxation approximates the convex hull of the feasible solutions to the program. To this end, it is important to choose \(M\) to be as small as possible.

There is no difficulty in incorporating additional linear equations and inequalities; in fact, such constraints are likely to make the problem easier to solve as the feasible region of the relaxation is restricted. This observation also indicates the value of incorporating the unnecessary constraints \(v_1 \leq v_2 \leq \cdots \leq v_k\). Typical integer linear-programming solution methods will prefer solutions with many inequalities active, when multiple solutions exist. For example, we might consider restricting \(s\) to be nonnegative (thereby forcing the center to lie in the convex hull of the points), in which
case the solution methods will tend to prefer those with coordinates of \( s \) equal to zero, when such solutions exist.

One possible way to find a suitable value for \( M \) is to solve the \( n(n - 1) \) linear programs

\[
m_{ij} = \max(w_i - w_j)
\]

s.t. \( Ds = w, \quad e^T s = 1, \quad w, s \in \mathbb{R}^n, \)

where \( i \) and \( j \) are distinct indices. Then \( M := \max\{m_{ij}\} \). This strategy is guaranteed to work if the feasible region is bounded; for example, requiring \( s \geq 0 \) would force \( M \) to take a finite value.

It is also worth noting that the difficulty in solving the program is driven by the number of binary variables; hence, it is easier to discover the optimal value \( k^* \) when it is small.

The following example illustrates that the above method may have multiple solutions, which in turn illustrate various parts of the theory. Suppose we have six points in the plane on two spheres with center the origin whose coordinates are \((1, 0), (-1, 0), (0, -1), (2, 0), (0, 2), (-2, 0)\). The corresponding distance matrix is given by

\[
D = \begin{bmatrix}
0 & 4 & 2 & 1 & 5 & 9 \\
4 & 0 & 2 & 9 & 5 & 1 \\
2 & 2 & 0 & 5 & 9 & 5 \\
1 & 9 & 5 & 0 & 8 & 16 \\
5 & 5 & 9 & 8 & 0 & 5 \\
9 & 1 & 5 & 16 & 8 & 0 \\
\end{bmatrix}.
\]

The following vectors \( s \) were obtained, and the vector \( Ds \) indicates that two blocks exist or that the points lie on two spheres:

\[
\begin{align*}
(1) \quad s &= \begin{bmatrix} \frac{3}{2}, \frac{1}{6}, 0, -\frac{2}{3}, 0, 0 \end{bmatrix}^T, \quad Ds = \begin{bmatrix} 0, 0, 0, 3, 3, 3 \end{bmatrix}^T, \\
(2) \quad s &= \begin{bmatrix} \frac{1}{2}, \frac{1}{3}, 0, 0, 0, 0 \end{bmatrix}^T, \quad Ds = \begin{bmatrix} 2, 2, 2, 5, 5, 5 \end{bmatrix}^T, \\
(3) \quad s &= \begin{bmatrix} \frac{1}{4}, \frac{1}{4}, 0, \frac{1}{4}, 0, \frac{1}{4} \end{bmatrix}^T, \quad Ds = \begin{bmatrix} \frac{7}{2}, \frac{7}{2}, \frac{13}{2}, \frac{13}{2}, \frac{13}{2} \end{bmatrix}^T.
\end{align*}
\]

The first case indicates the two-block structure. In the second case since the vector \( s \) has nonnegative components, the origin is in the convex hull of each spherical cluster of points. In the third case the vector \( s \) satisfies the conditions of Theorem 4.2. If \( S \) denotes the diagonal matrix whose diagonals are the elements of \( s \), then in case (1) \( DS \) has no block eigenvectors, and in case (2) it has one block eigenvector. In case (3), \( DS \) has two block eigenvectors, each consisting of two blocks of length three, as predicted by part (c) of Theorem 4.2.
A second example illustrates that there may be alternative choices of spheres that obtain the minimal number. We take the four standard unit vectors on the unit circle and two points on the circle with center the origin and radius \( \sqrt{17} \). The coordinates are \((0, 1), (0, -1), (1, 0), (-1, 0), (4, 1), (4, -1)\). The algorithm found two solutions, the first being the expected four unit vectors on one circle and the remaining two on the second circle. We failed to see a second solution until the algorithm found the solution \( s = \begin{bmatrix} \frac{9}{8} & -\frac{9}{8} & 0 & -\frac{3}{8} \end{bmatrix}^T \) and \( D_s = w = \begin{bmatrix} -8 & 0 & -8 & 0 & -8 & 0 \end{bmatrix}^T \), which indicates points \((0, -1), (1, 0), (4, -1)\) are on one circle and the remaining points on another. Inspection reveals that the center is at \((2, -2)\). By symmetry there is another solution with center at \((2, 2)\).

We have recently learned that David Carlson and Charles R. Johnson have also addressed the problem of finding the minimal number of spheres by a different approach.

REFERENCES


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