Methods for Constructing Distance Matrices and the Inverse Eigenvalue Problem

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Abstract

Let $D_1 \in \mathbf{R}^{k\times k}$ and $D_2 \in \mathbf{R}^{l\times l}$ be two distance matrices. We provide necessary conditions on $Z \in \mathbf{R}^{k\times l}$ in order that $D = \begin{bmatrix} D_1 & Z \\ Z^T & D_2 \end{bmatrix} \in \mathbf{R}^{n\times n}$ be a distance matrix. We then show that it is always possible to border an $n\times n$ distance matrix, with certain scalar multiples of its Perron eigenvector, to construct an $(n+1)\times(n+1)$ distance matrix. We also give necessary and sufficient conditions for two principal distance matrix blocks D_1 and D_2 be used to form a distance matrix as above, where Z is a scalar multiple of a rank one matrix, formed from their Perron eigenvectors. Finally, we solve the inverse eigenvalue problem for distance matrices in certain special cases, including $n = 3, 4, 5, 6$, any n for which there exists a Hadamard matrix, and some other cases.

1. Introduction

A matrix $D = (d_{ij}) \in \mathbf{R}^{n\times n}$ is said to be a (squared) distance matrix if there are vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n \in \mathbf{R}^r$ $(1 \le r \le n)$ such that $d_{ij} = ||\mathbf{x}_i - \mathbf{x}_j||^2$, for all $i, j = 1, 2, \ldots, n$, where $||\cdot||$ denotes the Euclidean norm. Note that this definition allows the $n\times n$ zero distance matrix. Because of its centrality in formulating our results, we begin Section 2 with a theorem of Crouzeix and Ferland [4]. Our proof reorganizes and simplifies their argument and, in addition, corrects a gap in their argument that C2 implies C1 (see below). We then show in Section 3 that this theorem implies some necessary conditions on the block matrix Z, in order that two principal distance matrix blocks D_1 and D_2 can be used to construct the distance matrix $D = \begin{bmatrix} D_1 & Z \\ Z^T & D_2 \end{bmatrix} \in \mathbf{R}^{n\times n}$. A different approach has been been considered by Bakonyi and Johnson [1], where they show that if a partial distance matrix has a chordal graph (a matrix with two principal distance matrix blocks has a chordal graph), then there is a one entry at a time procedure to complete the matrix to a distance matrix. Generally, graph theoretic techniques were employed in these studies, following similar methods used in the completion of positive semidefinite matrices. In Section 4, we use Fiedler's construction of nonnegative symmetric matrices [6] to show that an $n\times n$ distance matrix can always be bordered with certain scalar multiples of its Perron eigenvector, to form an $(n+1)\times(n+1)$ distance matrix. Further, starting with two principal distance matrix blocks D_1 and D_2, we give necessary and sufficient conditions on Z, where Z is a rank one matrix formed from the Perron eigenvectors, in order that $D = \begin{bmatrix} D_1 & Z \\ Z^T & D_2 \end{bmatrix} \in \mathbf{R}^{n\times n}$ be a distance matrix. Finally, in Section 5, we show that if a symmetric matrix has eigenvector $\mathbf{e} = (1, 1, \ldots, 1)^T$, just one positive eigenvalue and zeroes on the diagonal, then it is a distance matrix. It will follow that by performing an orthogonal similarity of a trace zero, diagonal matrix with (essentially) a Hadamard matrix, where the diagonal matrix has just one positive eigenvalue, we obtain a distance matrix. We show then that the above methods lead, in some special cases, to a solution of the inverse eigenvalue problem for distance matrices. That is, given one nonnegative real number and $n-1$ nonpositive real numbers, with the sum of these n numbers equal to zero, can one contruct a distance matrix with these numbers as its eigenvalues? We will, as usual, denote by $\mathbf{e}_i$ the vector with a one in the ith position and zeroes elsewhere.

2. Almost positive semidefinite matrices

A symmetric matrix A is said to be almost positive semidefinite (or conditionally positive semidefinite) if $\mathbf{x}^T A\mathbf{x} \geq 0$, for all $\mathbf{x} \in \mathbf{R}^n$ such that $\mathbf{x}^T\mathbf{e} = 0$. Theorem 2.1 gives some useful equivalent conditions in the theory of almost positive semidefinite matrices.

Theorem 2.1 (Crouzeix, Ferland) Let $A \in \mathbf{R}^{n\times n}$ be symmetric, and $\mathbf{a} \in \mathbf{R}^n, \mathbf{a} \neq 0$. Then the following are equivalent:

C1. $\mathbf{h}^T\mathbf{a} = 0$ implies $\mathbf{h}^T A\mathbf{h} \geq 0$.

C2. A is positive semidefinite *or* A has just one negative eigenvalue and there exists $\mathbf{b} \in \mathbf{R}^n$ such that $A\mathbf{b} = \mathbf{a}$, where $\mathbf{b}^T\mathbf{a} \leq 0$.

C3. The bordered matrix $\begin{bmatrix} A & a \\ a^T & 0 \end{bmatrix}$ has just one negative eigenvalue.

Proof: C1 implies C2:

Since A is positive semidefinite on a subspace of dimension $n-1$, A has at most one negative eigenvalue.

If there doesn't exist $\mathbf{b} \in \mathbf{R}^n$ such that $A\mathbf{b} = \mathbf{a}$, then writing $\mathbf{a} = \mathbf{x}+\mathbf{y}$, where $\mathbf{x} \in \ker A$ and $\mathbf{y} \in \text{range}A$, we must have $\mathbf{x} \neq \mathbf{0}$. But then $\mathbf{x}^T\mathbf{a} = \mathbf{x}^T\mathbf{x} + \mathbf{x}^T\mathbf{y} = \mathbf{x}^T\mathbf{x} \neq 0$. For any $\mathbf{v} \in \mathbf{R}^n$, define $\mathbf{h} = (I - \frac{\mathbf{x}\mathbf{a}^T}{\mathbf{x}^T\mathbf{a}})\mathbf{v} = \mathbf{v} - \frac{\mathbf{a}^T\mathbf{v}}{\mathbf{x}^T\mathbf{a}}\mathbf{x}$, then $\mathbf{h}^T\mathbf{a} = 0$, and $\mathbf{h}^T A\mathbf{h} = \mathbf{v}^T A\mathbf{v} \geq 0$, so A is positive semidefinite.

Suppose A is not positive semidefinite, $A\mathbf{b} = \mathbf{a}$ and $\mathbf{b}^T\mathbf{a} \neq 0$. For $\mathbf{v} \in \mathbf{R}^n$, let $\mathbf{h} = (I - \frac{\mathbf{b}\mathbf{a}^T}{\mathbf{b}^T\mathbf{a}})\mathbf{v}$, thus we can write any $\mathbf{v} \in \mathbf{R}^n$ as $\mathbf{v} = \mathbf{h} + \frac{\mathbf{a}^T\mathbf{v}}{\mathbf{b}^T\mathbf{a}}\mathbf{b}$, where $\mathbf{h}^T\mathbf{a} = 0$. Then

$$\mathbf{v}^T A\mathbf{v} = \mathbf{h}^T A\mathbf{h} + 2\frac{\mathbf{a}^T\mathbf{v}}{\mathbf{b}^T\mathbf{a}}\mathbf{h}^T A\mathbf{b} + (\frac{\mathbf{a}^T\mathbf{v}}{\mathbf{b}^T\mathbf{a}})^2\mathbf{b}^T A\mathbf{b} \geq (\frac{\mathbf{a}^T\mathbf{v}}{\mathbf{b}^T\mathbf{a}})^2\mathbf{b}^T\mathbf{a},$$

and choosing $\mathbf{v}$ so that $0 > \mathbf{v}^T A\mathbf{v}$ we see that $0 > \mathbf{b}^T\mathbf{a}$.

C2 implies C1:

If A is positive semidefinite we're done. Otherwise, let λ be the negative eigenvalue of A, with unit eigenvector $\mathbf{u}$. Write $A = C^TC + \lambda\mathbf{u}\mathbf{u}^T$, so that $\mathbf{a} = A\mathbf{b} = C^TC\mathbf{b} + \lambda(\mathbf{u}^T\mathbf{b})\mathbf{u}$.

If $\mathbf{u}^T\mathbf{b} = 0$ then $0 \geq \mathbf{b}^T\mathbf{a} = \mathbf{b}^TC^TC\mathbf{b}$, which implies $C\mathbf{b} = \mathbf{0}$ but then $\mathbf{a} = \mathbf{0}$ also, contradicting the hypotheses of our theorem. So we must have $\mathbf{u}^T\mathbf{b} \neq 0$.

Again, $\mathbf{a} = C^TC\mathbf{b} + \lambda(\mathbf{u}^T\mathbf{b})\mathbf{u}$ gives $0 \geq \mathbf{b}^T\mathbf{a} = \mathbf{b}^TC^TC\mathbf{b} + \lambda(\mathbf{u}^T\mathbf{b})^2$, which we can rewrite as $-1 \leq \frac{\mathbf{b}^TC^TC\mathbf{b}}{\lambda(\mathbf{u}^T\mathbf{b})^2}$. Noting also that $\mathbf{u} = \frac{1}{\lambda(\mathbf{u}^T\mathbf{b})}[\mathbf{a} - C^TC\mathbf{b}]$, we have

$$A = C^TC + \frac{1}{\lambda(\mathbf{u}^T\mathbf{b})^2}[\mathbf{a} - C^TC\mathbf{b}][\mathbf{a} - C^TC\mathbf{b}]^T.$$

If $\mathbf{h}^T\mathbf{a} = 0$ then

$$\begin{aligned}
\mathbf{h}^TA\mathbf{h} &= \mathbf{h}^TC^TC\mathbf{h} + \frac{1}{\lambda(\mathbf{u}^T\mathbf{b})^2}(\mathbf{h}^TC^TC\mathbf{b})^2, \\
&\geq \mathbf{h}^TC^TC\mathbf{h} - \frac{(\mathbf{h}^TC^TC\mathbf{b})^2}{\mathbf{b}^TC^TC\mathbf{b}}, \\
&= ||C\mathbf{h}||^2 - \frac{[(C\mathbf{h})^T(C\mathbf{b})]^2}{||C\mathbf{b}||^2} \geq 0,
\end{aligned}$$

where the last inequality is from Cauchy-Schwarz.

Finally, if $\mathbf{b}^TC^TC\mathbf{b} = 0$ then $C\mathbf{b} = 0$ which implies $\mathbf{a} = \lambda(\mathbf{u}^T\mathbf{b})\mathbf{u}$. Then $\mathbf{h}^T\mathbf{a} = 0$ implies $\mathbf{h}^T\mathbf{u} = 0$, so that $\mathbf{h}^TA\mathbf{h} = \mathbf{h}^T(C^TC + \lambda\mathbf{u}\mathbf{u}^T)\mathbf{h} = \mathbf{h}^TC^TC\mathbf{h} \geq 0$, as required.

The equivalence of C1 and C3 was proved by Ferland in [5].

Schoenberg [15] (see also Blumenthal [2,p106]) showed that a symmetric matrix $D = (d_{ij}) \in \mathbf{R}^{n\times n}$ (with $d_{ii} = 0,\ 1 \leq i \leq n$) is a distance matrix if and only if $\mathbf{x}^TD\mathbf{x} \leq 0$, for all $\mathbf{x} \in \mathbf{R}^n$ such that $\mathbf{x}^T\mathbf{e} = 0$.

Note that D almost negative semidefinite with zeroes on the diagonal implies that D is a nonnegative matrix, since $(\mathbf{e}_i - \mathbf{e}_j)^T\mathbf{e} = 0$ and so $(\mathbf{e}_i - \mathbf{e}_j)^TD(\mathbf{e}_i - \mathbf{e}_j) = -2d_{ij} \leq 0$.

Let $\mathbf{s} \in \mathbf{R}^n$, where $\mathbf{s}^T\mathbf{e} = 1$. Gower [7] proved that D is a distance matrix if and only if $(I - \mathbf{e}\mathbf{s}^T)D(I - \mathbf{s}\mathbf{e}^T)$ is negative semidefinite. (This follows since for any $\mathbf{y} \in \mathbf{R}^n$, $\mathbf{x} = (I - \mathbf{s}\mathbf{e}^T)\mathbf{y}$ is orthogonal to $\mathbf{e}$. Conversely, if $\mathbf{x}^T\mathbf{e} = 0$ then $\mathbf{x}^T(I - \mathbf{e}\mathbf{s}^T)D(I - \mathbf{s}\mathbf{e}^T)\mathbf{x} = \mathbf{x}^TD\mathbf{x}$.) The vectors from the origin to the n vertices are the columns of $X \in \mathbf{R}^{n\times n}$ in $(I - \mathbf{e}\mathbf{s}^T)\frac{1}{2}D(I - \mathbf{s}\mathbf{e}^T) = -X^TX$. (This last fact follows by writing $-2X^TX = (I - \mathbf{e}\mathbf{s}^T)D(I - \mathbf{s}\mathbf{e}^T) = D - \mathbf{f}\mathbf{e}^T - \mathbf{e}\mathbf{f}^T$, where $\mathbf{f} = D\mathbf{s} - \frac{1}{2}(\mathbf{s}^TD\mathbf{s})$, then $-2(\mathbf{e}_i - \mathbf{e}_j)^TX^TX(\mathbf{e}_i - \mathbf{e}_j) = (\mathbf{e}_i - \mathbf{e}_j)^TD(\mathbf{e}_i - \mathbf{e}_j) = d_{ii} + d_{jj} - 2d_{ij} = -2d_{ij}$, so that $d_{ij} = ||X\mathbf{e}_i - X\mathbf{e}_j||^2$.)

These results imply a useful theorem for later sections (see also [7], [18]).

Theorem 2.2 Let $D = (d_{ij}) \in \mathbf{R}^{n\times n}$, with $d_{ii} = 0$, for all $i,\ \ 1 \leq i \leq n$, and suppose that D is not the zero matrix. Then D is a distance matrix if and only if D has just one positive eigenvalue and there exists $\mathbf{w} \in \mathbf{R}^n$ such that $D\mathbf{w} = \mathbf{e}$ and $\mathbf{w}^T\mathbf{e} \geq 0$.

Proof: This follows from taking $A = -D$ and $\mathbf{a} = \mathbf{e}$ in Theorem 2.1, Schoenberg's result, and the fact that $d_{ii} = 0$, for all i, $1 \leq i \leq n$, implies D can't be negative semidefinite.

Remark: Observe that if there are two vectors $\mathbf{w}_1, \mathbf{w}_2 \in \mathbf{R}^n$ such that $D\mathbf{w}_1 = D\mathbf{w}_2 = \mathbf{e}$, then $\mathbf{w}_1 - \mathbf{w}_2 = \mathbf{u} \in \ker(D)$, and so $\mathbf{e}^T\mathbf{w}_1 - \mathbf{e}^T\mathbf{w}_2 = \mathbf{e}^T\mathbf{u}$. But $\mathbf{e}^T\mathbf{u} = \mathbf{w}_1^T D\mathbf{u} = 0$, so we can conclude that $\mathbf{w}_1^T\mathbf{e} = \mathbf{w}_2^T\mathbf{e}$.

3. Construction of distance matrices.

Let $D_1 \in \mathbf{R}^{k\times k}$ be a nonzero distance matrix, and $D_2 \in \mathbf{R}^{l\times l}$ a distance matrix. Of course, thinking geometrically, there are many choices for $Z \in \mathbf{R}^{k\times l}$, $k + l = n$, such that $D = \begin{bmatrix} D_1 & Z \\ Z^T & D_2 \end{bmatrix} \in \mathbf{R}^{n\times n}$ persists in being a distance matrix. Our first theorem provides some necessary conditions that any such Z must satisfy.

Theorem 3.1 If Z is chosen so that D is a distance matrix, then $Z = D_1W$, for some $W \in \mathbf{R}^{k\times l}$. Further, $D_2 - W^TD_1W$ is negative semidefinite.

Proof: Let $Z\mathbf{e}_i = \mathbf{z}_i$, $1 \leq i \leq l$. Since $D = \begin{bmatrix} D_1 & Z \\ Z^T & D_2 \end{bmatrix}$ is a distance matrix then the $(k+1)\times(k+1)$ bordered matrix $S_i = \begin{bmatrix} D_1 & z_i \\ z_i^T & 0 \end{bmatrix}$ is a distance matrix also, for $1 \leq i \leq l$. This implies that S_i has just one positive eigenvalue, and so $\mathbf{z}_i = D_1\mathbf{w}_i$, using condition C3 in Theorem 2.1. Thus $Z = D_1W$, where $W\mathbf{e}_i = \mathbf{w}_i$, $1 \leq i \leq l$.

The last part follows from the identity

$$\begin{bmatrix} D_1 & D_1W \\ W^TD_1 & D_2 \end{bmatrix} = \begin{bmatrix} I & 0 \\ W^T & I \end{bmatrix} \begin{bmatrix} D_1 & 0 \\ 0 & D_2 - W^TD_1W \end{bmatrix} \begin{bmatrix} I & W \\ 0 & I \end{bmatrix},$$

and Sylvester's theorem [9], since the matrix on the left and D_1 on the right both have just one positive eigenvalue.

Remark: In claiming D_1 is a nonzero distance matrix this means that $k \geq 2$. If D_1 happened to be a zero distance matrix (for example when $k = 1$), then the off-diagonal block Z need not necessarily be in the range of that zero D_1 block. In the proof above if S_i has just one positive eigenvalue we can only apply C3 and conclude that $\mathbf{z}_i = D_1\mathbf{w}_i$ when D_1 is not negative semidefinite (i.e. when D_1 is not a zero distance matrix). The converse of Theorem 3.1 is not necessarily true, since consider the case where $l = 1$, $S = \begin{bmatrix} D_1 & z \\ z^T & 0 \end{bmatrix}$ and $\mathbf{z} = D_1\mathbf{w}$, with $\mathbf{w}^TD_1\mathbf{w} \geq 0$. We will see in the next section that if $\mathbf{z}$ is the Perron eigenvector for D_1, only certain scalar multiples of $\mathbf{z}$ will cause S to be a distance matrix.

If D_1 and D_2 are both nonzero distance matrices then we can state Theorem 3.1 in the following form, where the same proof works with the rows of Z.

Theorem 3.2 If Z is chosen so that D is a distance matrix, then $Z = D_1W = VD_2$, for some W, $V \in \mathbf{R}^{k\times l}$. Further, $D_2 - W^TD_1W$ and $D_1 - VD_2V^T$ are both negative semidefinite.

4. Using the Perron vector to construct a distance matrix.

As a consequence of the Perron-Frobenius Theorem [9], since a distance matrix has all nonnegative entries then it has a real eigenvalue $r \geq |\lambda|$ for all eigenvalues λ of D. Furthermore, the eigenvector that corresponds to r has nonnegative entries. We will use the notation that the vector $\mathbf{e}$ takes on the correct number of components depending on the context.

Theorem 4.1 Let $D \in \mathbf{R}^{n\times n}$ be a nonzero distance matrix with $D\mathbf{u} = r\mathbf{u}$, where r is the Perron eigenvalue and $\mathbf{u}$ is a unit Perron eigenvector. Let $D\mathbf{w} = \mathbf{e}$, $\mathbf{w}^T\mathbf{e} \geq 0$ and $\rho > 0$. Then the bordered matrix $\hat{D} = \begin{bmatrix} D & \rho u \\ \rho u^T & 0 \end{bmatrix}$ is a distance matrix if and only if ρ lies in the interval $[\alpha^-, \alpha^+]$, where $\alpha^{\pm} = \dfrac{r}{\mathbf{u}^T\mathbf{e} \mp \sqrt{r\mathbf{e}^T\mathbf{w}}}$.

Proof: We first show that $\hat{D}$ has just one positive eigenvalue and $\mathbf{e}$ is in the range of $\hat{D}$. From [6] the set of eigenvalues of $\hat{D}$ consists of the $n-1$ nonpositive eigenvalues of D, as well as the two eigenvalues of the 2×2 matrix $\begin{bmatrix} r & \rho \\ \rho & 0 \end{bmatrix}$, namely $\dfrac{r \pm \sqrt{r^2 + 4\rho^2}}{2}$. Thus $\hat{D}$ has just one positive eigenvalue. It is easily checked that $\hat{D}\hat{\mathbf{w}} = \mathbf{e}$ if

$$\hat{\mathbf{w}} = \begin{bmatrix} \mathbf{w} - (\frac{\mathbf{u}^T\mathbf{e}}{r} - \frac{1}{\rho})\mathbf{u} \\ \frac{1}{\rho}(\mathbf{u}^T\mathbf{e} - \frac{r}{\rho}) \end{bmatrix}.$$

It remains to determine for which values of ρ we have $\mathbf{e}^T\hat{\mathbf{w}} \geq 0$, i.e.

$$\mathbf{e}^T\mathbf{w} - \frac{1}{r}(\mathbf{u}^T\mathbf{e})^2 + \frac{2}{\rho}(\mathbf{u}^T\mathbf{e}) - \frac{r}{\rho^2} = \frac{1}{r}[\mathbf{u}^T\mathbf{e} - \sqrt{r(\mathbf{e}^T\mathbf{w})} - \frac{r}{\rho}][-\mathbf{u}^T\mathbf{e} - \sqrt{r(\mathbf{e}^T\mathbf{w})} + \frac{r}{\rho}] \geq 0.$$

After multiplying across by ρ^2, we see that this inequality holds precisely when ρ is between the two roots $\alpha^{\pm} = \dfrac{r}{\mathbf{u}^T\mathbf{e} \mp \sqrt{r\mathbf{e}^T\mathbf{w}}}$ of the quadratic. We can be sure of the existence of $\rho > 0$ by arguing as follows. $D\mathbf{w} = \mathbf{e}$ implies $\mathbf{u}^T D\mathbf{w} = r\mathbf{u}^T\mathbf{w} = \mathbf{u}^T\mathbf{e}$. Also, $D = r\mathbf{u}\mathbf{u}^T + \lambda_2\mathbf{u}_2\mathbf{u}_2^T + \cdots$ (the spectral decomposition of D) implies $\mathbf{w}^T\mathbf{e} = \mathbf{w}^T D\mathbf{w} = r(\mathbf{w}^T\mathbf{u})^2 + \lambda_2(\mathbf{w}^T\mathbf{u}_2)^2 + \cdots < r(\mathbf{w}^T\mathbf{u})^2$, i.e. $\mathbf{w}^T\mathbf{e} < r(\frac{\mathbf{u}^T\mathbf{e}}{r})^2 = \frac{(\mathbf{u}^T\mathbf{e})^2}{r}$, so that $(\mathbf{u}^T\mathbf{e})^2 > r\mathbf{w}^T\mathbf{e}$, which completes the proof.

Example: Let D be the distance matrix which corresponds to a unit square in the plane, then $D\mathbf{e} = 4\mathbf{e}$. In this case, $\alpha^- = 1$, $\alpha^+ = \infty$, and the new figure that corresponds to $\hat{D} = \begin{bmatrix} D & \rho u \\ \rho u^T & 0 \end{bmatrix}$, for $\rho \in [\alpha^-, \alpha^+]$, has an additional point on a ray through the center of the square and perpendicular to the plane.

Fiedler's construction also leads to a more complicated version of Theorem 4.1.

Theorem 4.2 Let $D_1 \in \mathbf{R}^{k\times k}$, $D_2 \in \mathbf{R}^{l\times l}$ be nonzero distance matrices with $D_1\mathbf{u} = r_1\mathbf{u}$, $D_2\mathbf{v} = r_2\mathbf{v}$, where r_1 and r_2 are the Perron eigenvalues of D_1 and D_2 respectively. Likewise,

$\mathbf{u}$ and $\mathbf{v}$ are the corresponding unit Perron eigenvectors. Let $D_1\mathbf{w}_1 = \mathbf{e}$, where $\mathbf{w}_1^T\mathbf{e} \geq 0$, $D_2\mathbf{w}_2 = \mathbf{e}$, where $\mathbf{w}_2^T\mathbf{e} \geq 0$, and $\rho > 0$ with $\rho^2 \neq r_1r_2$.

Then the matrix $\hat{D} = \begin{bmatrix} D_1 & \rho uv^T \\ \rho vu^T & D_2 \end{bmatrix}$ is a distance matrix if and only if $\rho^2 > r_1r_2$, $[(\mathbf{u}^T\mathbf{e})^2 - r_1\mathbf{e}^T\mathbf{w}_1 - r_1\mathbf{e}^T\mathbf{w}_2][(\mathbf{v}^T\mathbf{e})^2 - r_2\mathbf{e}^T\mathbf{w}_1 - r_2\mathbf{e}^T\mathbf{w}_2)] \geq 0$ and ρ is in the interval $[\alpha^-, \alpha^+]$, where

$$\alpha^{\pm} = \frac{(\mathbf{u}^T\mathbf{e})(\mathbf{v}^T\mathbf{e}) \pm \sqrt{[(\mathbf{u}^T\mathbf{e})^2 - r_1\mathbf{e}^T\mathbf{w}_1 - r_1\mathbf{e}^T\mathbf{w}_2][(\mathbf{v}^T\mathbf{e})^2 - r_2\mathbf{e}^T\mathbf{w}_1 - r_2\mathbf{e}^T\mathbf{w}_2)]}}{\frac{(\mathbf{u}^T\mathbf{e})^2}{r_1} + \frac{(\mathbf{v}^T\mathbf{e})^2}{r_2} - \mathbf{e}^T\mathbf{w}_1 - \mathbf{e}^T\mathbf{w}_2}$$

Proof: Fiedler's results show that the eigenvalues of $\hat{D}$ are the nonpositive eigenvalues of D_1 together with the nonpositive eigenvalues of D_2, as well as the two eigenvalues of $\begin{bmatrix} r_1 & \rho \\ \rho & r_2 \end{bmatrix}$. The latter two eigenvalues are $\frac{r_1+r_2 \pm \sqrt{(r_1+r_2)^2+4[\rho^2-r_1r_2]}}{2}$. Thus if $\rho^2 - r_1r_2 > 0$ then $\hat{D}$ has just one positive eigenvalue. Conversely, if $\hat{D}$ has just one positive eigenvalue then $0 \geq r_1 + r_2 - \sqrt{(r_1+r_2)^2 + 4[\rho^2 - r_1r_2]}$, which implies $(r_1+r_2)^2 + 4[\rho^2 - r_1r_2] \geq (r_1+r_2)^2$, i.e. $\rho^2 - r_1r_2 \geq 0$, but $\rho^2 - r_1r_2 \neq 0$ so $\rho^2 - r_1r_2 > 0$. Also, $\hat{D}\hat{\mathbf{w}} = \mathbf{e}$ where

$$\hat{\mathbf{w}} = \begin{bmatrix} \mathbf{w_1} + \frac{\rho}{r_1r_2-\rho^2}[\frac{\rho}{r_1}(\mathbf{u}^T\mathbf{e}) - \mathbf{v}^T\mathbf{e}]\mathbf{u} \\ \mathbf{w_2} + \frac{\rho}{r_1r_2-\rho^2}[\frac{\rho}{r_2}(\mathbf{v}^T\mathbf{e}) - \mathbf{u}^T\mathbf{e}]\mathbf{v} \end{bmatrix}.$$

Then using this $\hat{\mathbf{w}}$ we have

$$\mathbf{e}^T\hat{\mathbf{w}} = \mathbf{e}^T\mathbf{w}_1 + \mathbf{e}^T\mathbf{w}_2 + \frac{\rho}{r_1r_2 - \rho^2}[\frac{\rho}{r_1}(\mathbf{u}^T\mathbf{e})^2 + \frac{\rho}{r_2}(\mathbf{v}^T\mathbf{e})^2 - 2(\mathbf{u}^T\mathbf{e})(\mathbf{v}^T\mathbf{e})] \geq 0,$$

which we can rewrite, on multiplying across by $r_1r_2 - \rho^2$, as

$$(\mathbf{e}^T\mathbf{w}_1 + \mathbf{e}^T\mathbf{w}_2)r_1r_2 - 2\rho(\mathbf{u}^T\mathbf{e})(\mathbf{v}^T\mathbf{e}) + \rho^2[\frac{(\mathbf{u}^T\mathbf{e})^2}{r_1} + \frac{(\mathbf{v}^T\mathbf{e})^2}{r_2} - \mathbf{e}^T\mathbf{w}_1 - \mathbf{e}^T\mathbf{w}_2] \leq 0.$$

After some simplification the roots of this quadratic turn out to be

$$\alpha^{\pm} = \frac{(\mathbf{u}^T\mathbf{e})(\mathbf{v}^T\mathbf{e}) \pm \sqrt{[(\mathbf{u}^T\mathbf{e})^2 - r_1\mathbf{e}^T\mathbf{w}_1 - r_1\mathbf{e}^T\mathbf{w}_2))][(\mathbf{v}^T\mathbf{e})^2 - r_2\mathbf{e}^T\mathbf{w}_1 - r_2\mathbf{e}^T\mathbf{w}_2)]}}{\frac{(\mathbf{u}^T\mathbf{e})^2}{r_1} + \frac{(\mathbf{v}^T\mathbf{e})^2}{r_2} - \mathbf{e}^T\mathbf{w}_1 - \mathbf{e}^T\mathbf{w}_2}.$$

We saw in the proof of Theorem 4.1 that $\mathbf{e}^T\mathbf{w}_1 < \frac{(\mathbf{u}^T\mathbf{e})^2}{r_1}$ and $\mathbf{e}^T\mathbf{w}_2 < \frac{(\mathbf{v}^T\mathbf{e})^2}{r_2}$. The proof is complete once we note that that the discriminant of the quadratic is greater than or equal to zero precisely when $\mathbf{e}^T\hat{\mathbf{w}} \geq 0$ for some ρ.

Remark: The case $\rho = \sqrt{r_1r_2}$ is dealt with separately. In this case if $\hat{D}\hat{\mathbf{w}} = \mathbf{e}$, then it can be checked that $\frac{\mathbf{u}^T\mathbf{e}}{\sqrt{r_1}} = \frac{\mathbf{v}^T\mathbf{e}}{\sqrt{r_2}}$. Also $\hat{D}\hat{\mathbf{w}} = \mathbf{e}$, if we take $\hat{\mathbf{w}} = \begin{bmatrix} w_1 - \frac{u^Te}{r_1+r_2}u \\ w_2 - \frac{v^Te}{r_1+r_2}v \end{bmatrix}$, where $D_1\mathbf{w}_1 = \mathbf{e}$ and $D_2\mathbf{w}_2 = \mathbf{e}$. Then $\hat{D}$ is a distance matrix if and only if (for this $\hat{\mathbf{w}}$) $\hat{\mathbf{w}}^T\mathbf{e} \geq 0$.

5. The inverse eigenvalue problem for distance matrices.

Let $\sigma = \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \subset \mathbf{C}$. The inverse eigenvalue problem for distance matrices is that of finding necessary and sufficient conditions that σ be the spectrum of a (squared) distance matrix D. Evidently, since D is symmetric $\sigma \subset \mathbf{R}$. We have seen that if $D \in \mathbf{R}^{n\times n}$

is a nonzero distance matrix then D has just one positive eigenvalue. Also, since the diagonal entries of D are all zeroes, we have $\text{trace}(D) = \sum_{i=1}^n \lambda_i = 0$.

The inverse eigenvalue problem for nonnegative matrices remains as one of the long-standing unsolved problems in matrix theory; see for instance [3],[10],[13]. Suleimanova [17] and Perfect [12] solved the inverse eigenvalue problem for nonnegative matrices in the special case where $\sigma \subset \mathbf{R}$, $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\sum_{i=1}^n \lambda_i \geq 0$. They showed that these conditions are sufficient for the construction of a nonnegative matrix with spectrum σ. Fiedler [6] went further and showed that these same conditions are sufficient even when the nonnegative matrix is required to be symmetric. From what follows it appears that these conditions are sufficient even if the nonnegative matrix is required to be a distance matrix (when $\sum_{i=1}^n \lambda_i = 0$). We will use the following lemma repeatedly.

Lemma 5.1 Let $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$, where $\sum_{i=1}^n \lambda_i = 0$. Then

$$(n-1)|\lambda_n| \geq \lambda_1 \qquad \text{and} \qquad (n-1)|\lambda_2| \leq \lambda_1.$$

Proof: These inequalities follow since $\lambda_1 = \sum_{i=2}^n |\lambda_i|$ and $|\lambda_2| \leq |\lambda_3| \leq \cdots \leq |\lambda_n|$.

Theorem 5.2 Let $\sigma = \{\lambda_1, \lambda_2, \lambda_3\} \subset \mathbf{R}$, with $\lambda_1 \geq 0 \geq \lambda_2 \geq \lambda_3$ and $\lambda_1 + \lambda_2 + \lambda_3 = 0$. Then σ is the spectrum of a distance matrix $D \in \mathbf{R}^{3\times 3}$.

Proof: Construct an isoceles triangle in the xy-plane with one vertex at the origin, and the other two vertices at $\left(\sqrt{\frac{\lambda_2}{4} + \sqrt{\frac{(\lambda_2+\lambda_3)\lambda_3}{2}}}, \pm\frac{\sqrt{-\lambda_2}}{2}\right)$. These vertices yield the distance matrix

$$D = \begin{bmatrix} 0 & -\lambda_2 & \sqrt{\frac{(\lambda_2+\lambda_3)\lambda_3}{2}} \\ -\lambda_2 & 0 & \sqrt{\frac{(\lambda_2+\lambda_3)\lambda_3}{2}} \\ \sqrt{\frac{(\lambda_2+\lambda_3)\lambda_3}{2}} & \sqrt{\frac{(\lambda_2+\lambda_3)\lambda_3}{2}} & 0 \end{bmatrix},$$

and it is easily verified that D has characteristic polynomial $(x-\lambda_2)(x-\lambda_3)(x+\lambda_2+\lambda_3) = x^3 - (\lambda_2\lambda_3 + \lambda_2^2 + \lambda_3^2)x + \lambda_2\lambda_3(\lambda_2+\lambda_3)$.

Note that $\frac{\lambda_2}{4} + \sqrt{\frac{(\lambda_2+\lambda_3)\lambda_3}{2}} = \frac{\lambda_2}{4} + \sqrt{\frac{-\lambda_1\lambda_3}{2}} \geq \frac{\lambda_2}{4} + \sqrt{\frac{\lambda_1^2}{4}} = \frac{\lambda_2+2\lambda_1}{4} = \frac{-\lambda_3+\lambda_1}{4} \geq 0$, which completes the proof.

Some distance matrices have $\mathbf{e}$ as their Perron eigenvector. These were discussed in [8], and were seen to correspond to vertices which form regular figures.

Lemma 5.3 Let $D \in \mathbf{R}^{n\times n}$ be symmetric, have zeroes on the diagonal, have just one nonnegative eigenvalue λ_1, and corresponding eigenvector $\mathbf{e}$. Then D is a distance matrix.

Proof: Let D have eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, then we can write $D = \dfrac{\lambda_1}{n}\mathbf{e}\mathbf{e}^T + \lambda_2\mathbf{u}_2\mathbf{u}_2^T + \cdots$. If $\mathbf{x}^T\mathbf{e} = 0$ then $\mathbf{x}^T D\mathbf{x} \leq 0$, as required.

A matrix $H \in \mathbf{R}^{n\times n}$ is said to be a Hadamard matrix if each entry is equal to ± 1 and $H^T H = nI$. These matrices exist only if $n = 1, 2$ or $n \equiv 0 \bmod 4$ [19]. It is not known if there exists a Hadamard matrix for every $n \geq 4$ which is a multiple of 4, although this is a well-known conjecture. Examples of Hadamard matrices are:

$$n = 2, \qquad H = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}; \qquad n = 4, \qquad H = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix};$$

and $H_1 \otimes H_2$ is a Hadamard matrix, where H_1 and H_2 are Hadamard matrices and $\otimes$ denotes the Kronecker product. For any n for which there exists a Hadamard matrix our next theorem solves the inverse eigenvalue problem.

Theorem 5.4 Let n be such that there exists a Hadamard matrix of order n. Let $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\sum_{i=1}^{n} \lambda_i = 0$. Then there is a distance matrix D with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$.

Proof: Let $H \in \mathbf{R}^{n\times n}$ be a Hadamard matrix, and $U = \frac{1}{\sqrt{n}} H$ so that U is an orthogonal matrix. Let $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_n)$, then $D = U^T \Lambda U$ has eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. D has eigenvector $\mathbf{e}$, since for any Hadamard matrix H we can assume that one of the columns of H is $\mathbf{e}$. From $D = U^T \Lambda U = \dfrac{\lambda_1}{n}\mathbf{e}\mathbf{e}^T + \lambda_2 \mathbf{u}_2 \mathbf{u}_2^T + \cdots$, it can be seen that each of the diagonal entries of D are $\sum_{i=1}^{n} \lambda_i / n = 0$. The theorem then follows from Lemma 5.3.

Since there are Hadamard matrices for all n a multiple of 4 such that $4 \leq n < 428$, Theorem 5.4 solves the inverse eigenvalue problem in these special cases. See [16] for a more extensive list of values of n for which there exists a Hadamard matrix. The technique of Theorem 5.4 was used in [10] to partly solve the inverse eigenvalue problem for nonnegative matrices when $n = 4$.

Theorem 5.6 will solve the inverse eigenvalue problem for any $n + 1$, such that there exists a Hadamard matrix of order n. We will use a theorem due to Fiedler [6].

Theorem 5.5 Let $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_k$ be the eigenvalues of the symmetric nonnegative matrix $A \in \mathbf{R}^{k\times k}$, and $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_l$ the eigenvalues of the symmetric nonnegative matrix $B \in \mathbf{R}^{l\times l}$, where $\alpha_1 \geq \beta_1$. Moreover, $A\mathbf{u} = \alpha_1 \mathbf{u}$, $B\mathbf{v} = \beta_1 \mathbf{v}$, so that $\mathbf{u}$ and $\mathbf{v}$ are the corresponding unit Perron eigenvectors. Then with $\rho = \sqrt{\sigma(\alpha_1 - \beta_1 + \sigma)}$ the matrix $\begin{bmatrix} A & \rho u v^T \\ \rho v u^T & B \end{bmatrix}$ has eigenvalues $\alpha_1 + \sigma, \beta_1 - \sigma, \alpha_2, \ldots, \alpha_k, \beta_2, \ldots, \beta_l$, for any $\sigma \geq 0$.

Remark: The assumption $\alpha_1 \geq \beta_1$ is only for convenience. It is easily checked that it is sufficient to have $\alpha_1 - \beta_1 + \sigma \geq 0$.

In [18] two of the authors called a distance matrix circum–Euclidean if the points which generate it lie on a hypersphere. Suppose that the distance matrix D has the property that there is an $\mathbf{s} \in \mathbf{R}^n$ such that $D\mathbf{s} = \beta\mathbf{e}$ and $\mathbf{s}^T\mathbf{e} = 1$ (easily arranged if $D\mathbf{w} = \mathbf{e}$ and $\mathbf{w}^T\mathbf{e} > 0$). Then using this $\mathbf{s}$ we have (see the paragraph just before Theorem 2.2)

$$(I - \mathbf{e}\mathbf{s}^T)D(I - \mathbf{s}\mathbf{e}^T) = D - \beta\mathbf{e}\mathbf{e}^T = -2X^TX.$$

Since the diagonal entries of D are all zero, if $X\mathbf{e}_i = \mathbf{x}_i$, then $||\mathbf{x}_i||^2 = \beta/2$, for all i, $1 \le i \le n$. Evidently the points lie on a hypersphere of radius R, where $R^2 = \beta/2 = \dfrac{\mathbf{s}^T D\mathbf{s}}{2}$.

Theorem 5.6 Let n be such that there exists a Hadamard matrix of order n. Let $\lambda_1 \ge 0 \ge \lambda_2 \ge \cdots \ge \lambda_{n+1}$ and $\sum_{i=1}^{n+1} \lambda_i = 0$, then there is an $(n+1) \times (n+1)$ distance matrix $\hat{D}$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{n+1}$.

Proof: Let $D \in \mathbf{R}^{n\times n}$ be a distance matrix constructed using a Hadamard matrix, as in Theorem 5.4, with eigenvalues $\lambda_1 + \lambda_{n+1}, \lambda_2, \ldots, \lambda_n$. Note that $\lambda_1 + \lambda_{n+1} = -\lambda_2 - \cdots - \lambda_n$ and $D\mathbf{e} = (\lambda_1 + \lambda_{n+1})\mathbf{e}$, i.e. D has Perron eigenvector $\mathbf{e}$. Using Theorem 5.5 let $\hat{D} = \begin{bmatrix} D & \rho u \\ \rho u^T & 0 \end{bmatrix}$, where $A = D$, $B = 0$, $\mathbf{u} = \frac{\mathbf{e}}{\sqrt{n}}$, $\alpha_1 = \lambda_1 + \lambda_{n+1}$, $\alpha_i = \lambda_i$, for $2 \le i \le n$, $\beta_1 = 0$ and $\sigma = -\lambda_{n+1}$. In this case $\rho = \sqrt{-\lambda_1\lambda_{n+1}}$, and $\hat{D}$ has eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{n+1}$. We will show that there exist vectors $\hat{\mathbf{x}}_1, \ldots, \hat{\mathbf{x}}_{n+1}$ such that $\hat{d}_{ij} = ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j||^2$, for all i, j, $1 \le i, j \le n+1$, where $\hat{D} = (\hat{d}_{ij})$.

For the distance matrix D, and in the notation of the paragraph above, $\mathbf{s} = \dfrac{\mathbf{e}}{n}$ and $\beta = \dfrac{(\lambda_1 + \lambda_{n+1})}{n}$. Let $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbf{R}^n$ be vectors to the n vertices that will correspond to D, i.e. $d_{ij} = ||\mathbf{x}_i - \mathbf{x}_j||^2$, for all i, j, $1 \le i, j \le n$. These points lie on a hypersphere of radius R, where $R^2 = ||\mathbf{x}_i||^2 = \dfrac{(\lambda_1 + \lambda_{n+1})}{2n}$, for all i, $1 \le i \le n$.

Let the vectors that correspond to the $n+1$ vertices of $\hat{D}$ be $\hat{\mathbf{x}}_1 = (\mathbf{x}_1, 0), \ldots, \hat{\mathbf{x}}_n = (\mathbf{x}_n, 0) \in \mathbf{R}^{n+1}$ and $\hat{\mathbf{x}}_{n+1} = (\mathbf{0}, t) \in \mathbf{R}^{n+1}$, then $\hat{d}_{ij} = d_{ij}$, for all i, j, $1 \le i, j \le n$. Furthermore, the right-most column of $\hat{D}$ has entries $\hat{d}_{i(n+1)} = ||\hat{\mathbf{x}}_{n+1} - \hat{\mathbf{x}}_i||^2 = t^2 + R^2$, for each i, $1 \le i \le n$.

Finally, we must show that we can choose t so that $t^2 + R^2 = \dfrac{\rho}{\sqrt{n}}$. But this will be possible only if $R^2 \le \dfrac{\rho}{\sqrt{n}}$, i.e. $\dfrac{(\lambda_1 + \lambda_{n+1})}{2n} \le \dfrac{\sqrt{-\lambda_1\lambda_{n+1}}}{\sqrt{n}}$, which we can rewrite, on dividing both sides by $\dfrac{\lambda_1}{n}$ as $\dfrac{1-p}{2} \le \sqrt{np}$, where $p = \dfrac{-\lambda_{n+1}}{\lambda_1}$. Since $p \ge 0$ we must have $\dfrac{1-p}{2} \le \dfrac{1}{2}$. But also, from Lemma 5.1, $p \ge \dfrac{1}{n}$ implies that $\sqrt{np} \ge 1$, and the proof is complete.

Note that the above proof works for any distance matrix D with eigenvector $\mathbf{e}$, and with the appropriate eigenvalues, not just when D has been constructed using a Hadamard matrix. The same is true for the matrix D_1 in our next theorem. Our next theorem bears a close resemblance to the previous one, although it will solve the inverse eigenvalue problem only in the cases $n = 6, 10, 14$ and 18.

Theorem 5.7 Let $n = 4, 8, 12$ or 16, so that there exists a Hadamard matrix of order n. Let $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_{n+1} \geq \lambda_{n+2}$ and $\sum_{i=1}^{n+2} \lambda_i = 0$, then there is an $(n+2) \times (n+2)$ distance matrix $\hat{D}$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{n+1}, \lambda_{n+2}$.

Proof: Let $D_1 \in \mathbf{R}^{n \times n}$ be a distance matrix, constructed using a Hadamard matrix as before, with eigenvalues $\lambda_1 + \lambda_{n+1} + \lambda_{n+2}, \lambda_2, \ldots, \lambda_n$. Let $\hat{D} = \begin{bmatrix} D_1 & \rho \frac{e}{\sqrt{n}} \frac{e^T}{\sqrt{2}} \\ \rho \frac{e}{\sqrt{n}} \frac{e^T}{\sqrt{2}} & D_2 \end{bmatrix}$, where $D_2 = \begin{bmatrix} 0 & -\lambda_{n+1} \\ -\lambda_{n+1} & 0 \end{bmatrix}$, and apply Theorem 5.5 where $A = D_1$, $B = D_2$, $\mathbf{u} = \frac{1}{\sqrt{n}}\mathbf{e}$, $\mathbf{v} = \frac{1}{\sqrt{2}}\mathbf{e}$, $\alpha_1 = \lambda_1 + \lambda_{n+1} + \lambda_{n+2}$, $\alpha_i = \lambda_i$, for $2 \leq i \leq n$, $\beta_1 = -\lambda_{n+1}$, $\beta_2 = \lambda_{n+1}$ and $\sigma = -\lambda_{n+1} - \lambda_{n+2}$. In this case $\rho = \sqrt{(-\lambda_{n+1} - \lambda_{n+2})(\lambda_1 + \lambda_{n+1})}$, and $\hat{D}$ has the desired eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{n+1}, \lambda_{n+2}$.

The vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ to the n vertices that correspond to D_1 lie on a hypersphere of radius $R^2 = \frac{\lambda_1 + \lambda_{n+1} + \lambda_{n+2}}{2n}$. Let the vectors that correspond to the $n+2$ vertices of $\hat{D}$ be $\hat{\mathbf{x}}_1 = (\mathbf{x}_1, 0, 0), \ldots, \hat{\mathbf{x}}_n = (\mathbf{x}_n, 0, 0) \in \mathbf{R}^{n+2}$ and $\hat{\mathbf{x}}_{n+1} = (\mathbf{0}, t, \frac{\sqrt{-\lambda_{n+1}}}{2})$, $\hat{\mathbf{x}}_{n+2} = (\mathbf{0}, t, -\frac{\sqrt{-\lambda_{n+1}}}{2}) \in \mathbf{R}^{n+2}$, then $\hat{d}_{ij} = ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j||^2 = ||\mathbf{x}_i - \mathbf{x}_j||^2$, for all i, j, $1 \leq i, j \leq n$, and $\hat{d}_{ij} = ||\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j||^2$, for $n+1 \leq i, j \leq n+2$. Furthermore, the rightmost two columns of $\hat{D}$ (excluding the entries of the bottom right 2×2 block) have entries $\hat{d}_{i(n+1)} = ||\hat{\mathbf{x}}_{n+1} - \hat{\mathbf{x}}_i||^2 = R^2 + t^2 - \dfrac{\lambda_{n+1}}{4} = \hat{d}_{i(n+2)} = ||\hat{\mathbf{x}}_{n+2} - \hat{\mathbf{x}}_i||^2$, for each i, $1 \leq i \leq n$.

Finally, we must show that we can choose t so that $R^2 + t^2 - \dfrac{\lambda_{n+1}}{4} = \dfrac{\rho}{\sqrt{n}\sqrt{2}}$, i.e. we must show that

$$\frac{\lambda_1 + \lambda_{n+1} + \lambda_{n+2}}{2n} - \frac{\lambda_{n+1}}{4} \leq \sqrt{\frac{(-\lambda_{n+1} - \lambda_{n+2})(\lambda_1 + \lambda_{n+1})}{2n}}.$$

Writing $p = \dfrac{-\lambda_{n+1}}{\lambda_1}$ and $q = \dfrac{-\lambda_{n+2}}{\lambda_1}$, we can rewrite the above inequality as

$$\frac{1 - p - q}{2n} + \frac{p}{4} \leq \sqrt{\frac{(p+q)(1-p)}{2n}}.$$

This inequality can be rearranged to become

$$\frac{1}{2n} + \frac{1}{4} \leq \frac{1-p}{4} + \frac{p+q}{2n} + \sqrt{\frac{(p+q)(1-p)}{2n}},$$

or

$$\frac{2+n}{4n} \leq [\sqrt{\frac{p+q}{2n}} + \frac{\sqrt{1-p}}{2}]^2,$$

then taking square roots of both sides and again rearranging, we have

$$1 \leq \sqrt{\frac{2}{2+n}}\sqrt{p+q} + \sqrt{\frac{n}{2+n}}\sqrt{1-p} = f(p,q).$$

Thus, we need to show that $f(p,q) \geq 1$, where $q \geq p$, $1 \geq p+q$, and $np \geq 1-q$ (the last inequality comes from noting that $\lambda_1 + \lambda_{n+2} \geq \lambda_2 \geq \cdots \geq \lambda_n \geq \lambda_{n+1}$, since $\sum_{i=1}^{n+2} \lambda_i = 0$, and using Lemma 5.1). These three inequalities describe the interior of a triangular region in the pq-plane. For fixed p, $f(p,q)$ increases as q increases, so we need only check that $f(p,q) \geq 1$, on the lower border (i.e. closest to the p-axis) of the triangular region. One edge of this lower border is when $p = q$, and in this case $\frac{1}{2} \geq p \geq \frac{1}{n+1}$. Differentiation of $f(p,p)$ tells us that a maximum is achieved when $p = \frac{4}{n+4}$, and $\frac{1}{2} \geq \frac{4}{n+4} \geq \frac{1}{n+1}$ since $n \geq 4$. Minima are achieved at the end-points $p = \frac{1}{2}$ and $p = \frac{1}{n+1}$. It is easily checked that $f(\frac{1}{2}, \frac{1}{2}) \geq 1$, means that $16 \geq n$, and that $f(\frac{1}{n+1}, \frac{1}{n+1}) \geq 1$ is true in any case. Along the other lower border $q = -np + 1$, and in this case $f(p, -np+1)$ is found to have $\frac{df}{dp} < 0$, and we're done since $f(\frac{1}{n+1}, \frac{1}{n+1}) \geq 1$.

The methods described above do not appear to extend to the missing cases, particularly the case of $n = 7$. Since we have no evidence that there are any other necessary conditions on the eigenvalues of a distance matrix we make the following conjecture:

Conjecture Let $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$, where $\sum_{i=1}^{n} \lambda_i = 0$. Then there is a distance matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$.

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