Properties of Euclidean and Non-Euclidean Distance Matrices

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ABSTRACT

A distance matrix $\mathbf{D}$ of order n is symmetric with elements $-\frac{1}{2}d_{ij}^2$, where $d_{ii}=0$. $\mathbf{D}$ is Euclidean when the $\frac{1}{2}n(n-1)$ quantities d_{ij} can be generated as the distances between a set of n points, $\mathbf{X}$ $(n\times p)$, in a Euclidean space of dimension p. The dimensionality of $\mathbf{D}$ is defined as the least value of $p=\text{rank}(\mathbf{X})$ of any generating $\mathbf{X}$; in general $p+1$ and $p+2$ are also acceptable but may include imaginary coordinates, even when $\mathbf{D}$ is Euclidean. Basic properties of Euclidean distance matrices are established; in particular, when $\rho=\text{rank}(\mathbf{D})$ it is shown that, depending on whether $\mathbf{e}^T\mathbf{D}^-\mathbf{e}$ is not or is zero, the generating points lie in either $p=\rho-1$ dimensions, in which case they lie on a hypersphere, or in $p=\rho-2$ dimensions, in which case they do not. (The notation $\mathbf{e}$ is used for a vector all of whose values are one.) When $\mathbf{D}$ is non-Euclidean its dimensionality $p=r+s$ will comprise r real and s imaginary columns of $\mathbf{X}$, and (r,s) are invariant for all generating $\mathbf{X}$ of minimal rank. Higher-ranking representations can arise only from $p+1=(r+1)+s$ or $p+1=r+(s+1)$ or $p+2=(r+1)+(s+1)$, so that not only are r,s invariant, but they are both minimal for all admissible representations $\mathbf{X}$.

1. INTRODUCTION

The motivation for the following arises from the statistical problems of multidimensional scaling and ordination. However, few of the results obtained have immediate statistical applications; rather it is felt that these results have an intrinsic interest and eventually may help a better understanding of the statistical methodology.

In multidimensional scaling, an observed positive symmetric matrix is to be approximated by the "pairwise" Euclidean (sometimes other Minkowski) distances generated by a set of points whose coordinates are to be estimated

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in a specified number of dimensions. There are two general classes of goodness-of-fit criteria. In *metric* multidimensional scaling the differences between observed and fitted distances are minimized according (in general) to some least-squares criterion; in *nonmetric* multidimensional scaling only the ordinal values of the entries in the observed matrix are to be approximately reproduced as measured by suitable criteria. The terms metric and nonmetric can be misleading in the context of multidimensional scaling, for in both cases a metric (usually Euclidean) is fitted to the data—the distinction refers to whether the goodness-of-fit criterion is of least-squares type (metric) or is ordinal (nonmetric). This is not the place to go into details; see e.g., [3, 4] for an introduction and further references.

A problem of metric multidimensional scaling with non-Euclidean observations is of direct relevance to the following. The question arises as to the existence of a maximum number of Euclidean dimensions that can be fitted, after which no further improvement is attainable. Gower [2] shows that a non-Euclidean matrix of order n has best Euclidean fit in no more than $n-2$ real Euclidean dimensions, but it is conjectured that the upper limit is near to the number of "real dimensions" in the data, which may be much less than $n-2$. With Euclidean data, the number of real dimensions is easily defined, but with non-Euclidean data, closer examination is needed to define exactly what is meant, and this is one of the aims of the paper. Those familiar with multidimensional scaling should note that, apart from setting a possible upper bound to the number of dimensions that can be fitted, this conjecture has little bearing on deciding the smallest number of dimensions required to give a good approximation to the data.

Before attempting detailed analysis of this class of statistical problems, the basic mathematical properties of distance matrices are required, but little seems available in the literature. The following is an attempt to provide some initial results. Incidentally the material on the g-circumhypersphere provides some new results on best-fitting circles and hyperspheres.

Throughout this paper we shall be concerned with a real symmetric $n \times n$ matrix $\mathbf{D}$ with elements $-\frac{1}{2}d_{ij}^2$ and with zero diagonal. When a set of n points can be found in a Euclidean space of some dimensionality such that all $\frac{1}{2}n(n-1)$ interdistances generate the values d_{ij}, $\mathbf{D}$ is said to be Euclidean. Writing $\mathbf{e}$ for a vector all of whose values are one, Schoenberg [5] showed that $\mathbf{D}$ is Euclidean iff

$$\mathbf{F} \equiv (\mathbf{I} - \mathbf{e}\mathbf{s}^T)\mathbf{D}(\mathbf{I} - \mathbf{s}\mathbf{e}^T) \tag{1}$$

is positive semi-definite (p.s.d.), where $\mathbf{s} = \mathbf{e}/n$ or $\mathbf{s} = \mathbf{e}_i$, a unit vector with zero everywhere except in the ith position. Gower [1] generalized this result to show that the result was true for any s such that $\mathbf{s}^T\mathbf{e} = 1$ and $\mathbf{Ds} \neq \mathbf{0}$, deriving the result *ab initio*. To derive the general result from Schoenberg's is trivial, for

$$\mathbf{F}_1 = \left(\mathbf{I} - \frac{\mathbf{ee}^T}{n}\right)\mathbf{D}\left(\mathbf{I} - \frac{\mathbf{ee}^T}{n}\right)$$
$$= \left(\mathbf{I} - \frac{\mathbf{ee}^T}{n}\right)\mathbf{F}\left(\mathbf{I} - \frac{\mathbf{ee}^T}{n}\right),$$

so that when $\mathbf{F}$ is p.s.d., so is $\mathbf{F}_1$. Conversely, because $\mathbf{F} = (\mathbf{I} - \mathbf{es}^T)\mathbf{F}_1(\mathbf{I} - \mathbf{se}^T)$, it follows that when $\mathbf{F}$ is not p.s.d., neither can $\mathbf{F}_1$ be.

The condition $\mathbf{Ds} \neq \mathbf{0}$ turns out to be superfluous, for if $\mathbf{Ds} = \mathbf{0}$ then

$$\mathbf{s}^T\mathbf{F}_1\mathbf{s} = (\mathbf{s}^T\mathbf{e})^2 \frac{\mathbf{e}^T\mathbf{De}}{n^2}.$$

Now $\mathbf{e}^T\mathbf{De} = \Sigma(-\frac{1}{2}d_{ij}^2) \leqslant 0$, with equality only when all distances are zero, a possibility we exclude. However, because $\mathbf{F}_1$ is p.s.d., $\mathbf{s}^T\mathbf{F}_1\mathbf{s} \geqslant 0$, so $\mathbf{s}^T\mathbf{e} = 0$, a result obtained less directly in Section 3 below. This shows that whenever $\mathbf{D}$ is Euclidean, then $\mathbf{s}^T\mathbf{e} = 1$ and $\mathbf{Ds} = \mathbf{0}$ are incompatible. If $\mathbf{D}$ is non-Euclidean, we shall see below that it is possible to find $\mathbf{s}$ such that $\mathbf{Ds} = \mathbf{0}$ with $\mathbf{s}^T\mathbf{e} = 1$; with this choice of $\mathbf{s}$, $\mathbf{F} = \mathbf{D}$ with zero trace, and hence $\mathbf{F}$ is not p.s.d., as is required for non-Euclidean $\mathbf{D}$.

If $\mathbf{F} = \mathbf{XX}^T$ is any decomposition of $\mathbf{F}$, then the rows of $\mathbf{X}$ give coordinates of points that generate the distances d_{ij}, and clearly $\mathbf{X}^T\mathbf{s} = \mathbf{0}$, so that $\mathbf{s}$ determines the position of the origin; the different decompositions give different orientations about this origin. Schoenberg's choices $\mathbf{s} = \mathbf{e}/n$ and $\mathbf{s} = \mathbf{e}_i$ place the origin at the centroid and at the ith point of the configuration of n points. Gower [1] discussed the geometrical significance of other choices of $\mathbf{s}$ and, when $\mathbf{D}$ is of full rank, found explicit formulae for placing the origin at the circumcenter, incenter, and also excenters of the configuration. In what follows it turns out that the circumhypersphere and its radius play a central role, so that for completeness, and to exhibit the development in its simplest form, the case when $\mathbf{D}$ is of full rank is reexamined.

From $\mathbf{F} = \mathbf{XX}^T$ it follows that the ith value of $\operatorname{diag}\mathbf{F}$ gives the squared distance of the ith point from the origin determined by $\mathbf{s}$. Now $\operatorname{diag}\mathbf{F}$ may be exhibited as the column vector:

$$(\mathbf{S}^T\mathbf{Ds})\mathbf{e} - 2\mathbf{Ds}. \tag{2}$$

This vector, then, gives the squared distances from the origin, and if this origin is to be the center of the circumhypersphere of radius R, then (2) must satisfy

$$(\mathbf{s}^T\mathbf{D}\mathbf{s})\mathbf{e} - 2\mathbf{D}\mathbf{s} = R^2\mathbf{e}, \tag{3}$$

which, since $\mathbf{D}$ is nonsingular, has solution

$$\mathbf{s} = k\mathbf{D}^{-1}\mathbf{e}$$

for some constant k. The existence of such a solution proves the existence of the circumhypersphere when $\det\mathbf{D} \neq 0$. The condition $\mathbf{s}^T\mathbf{e} = 1$ immediately determines k to give $\mathbf{s} = \mathbf{D}^{-1}\mathbf{e}/\mathbf{e}^T\mathbf{D}^{-1}\mathbf{e}$, which on substitution into (3) gives

$$R^2 = -(\mathbf{e}^T\mathbf{D}^{-1}\mathbf{e})^{-1},$$

indicating the additional requirement that $\mathbf{e}^T\mathbf{D}^{-1}\mathbf{e} \neq 0$ (see Section 3). This gives:

THEOREM 1. *If* $\mathbf{D}$ *is Euclidean,* $\det\mathbf{D} \neq 0$, *and* $\mathbf{e}^T\mathbf{D}^{-1}\mathbf{e} \neq 0$, *then a circumhypersphere exists with radius given by* $R^2 = -(\mathbf{e}^T\mathbf{D}^{-1}\mathbf{e})^{-1}$. *Coordinates* $\mathbf{X}$ *relative to the circumcenter may be found by setting* $\mathbf{s} = \mathbf{D}^{-1}\mathbf{e}/\mathbf{e}^T\mathbf{D}^{-1}\mathbf{e}$ *in* $\mathbf{F}$ *and using any decomposition* $\mathbf{F} = \mathbf{X}\mathbf{X}^T$.

Because R^2 is necessarily nonnegative it follows that:

COROLLARY. *When* $\mathbf{D}$ *is Euclidean and* $\det\mathbf{D} \neq 0$, *then* $\mathbf{e}^T\mathbf{D}^{-}\mathbf{e} \leqslant 0$.

A direct proof of the result seems difficult.

The following examines what happens when these conditions are successively relaxed. First we consider a $\mathbf{D}$ not of full rank, establish the condition for a circumhypersphere to exist, and examine the consequences of one definition of a best approximating hypersphere when an exact one does not exist. Then the relationship between the rank of $\mathbf{D}$ and the dimensionality of $\mathbf{X}$ is established, also the relationship between the null spaces of $\mathbf{F}$ and $\mathbf{D}$. Finally the condition that $\mathbf{F}$ is p.s.d. is relaxed, so that $\mathbf{X}$ may not be real and $\mathbf{D}$ may be non-Euclidean.

2. THE EXISTENCE OF A CIRCUMHYPERSPHERE

When $\mathbf{D}$ is not of full rank, the equations (3) may be inconsistent and have no solution. The points generating $\mathbf{D}$ then cannot lie on a hypersphere. An approximate circumcenter could then be defined in many ways, but it is convenient to work in terms of the deviations from the average squared distances from the origin, which are obtained immediately from (2) as

$$-2(\mathbf{I}-\mathbf{N})\mathbf{D}\mathbf{s}, \tag{4}$$

where $\mathbf{N}=\mathbf{e}\mathbf{e}^T/n$.

Definition. The g-circumcenter, a generalized circumcenter, is defined to be the origin given by the setting of $\mathbf{s}$ that minimizes the sums of squares of (4).

This sum of squares is $4\mathbf{s}^T\mathbf{D}(\mathbf{I}-\mathbf{N})\mathbf{D}\mathbf{s}$ and is to be minimized subject to $\mathbf{e}^T\mathbf{s}=1$. Thus we must solve

$$\mathbf{D}(\mathbf{I}-\mathbf{N})\mathbf{D}\mathbf{s}=\lambda\mathbf{e}, \tag{5}$$

where 4λ is the minimum sum of squares. When $\lambda=0$ the sum of squares of deviations is zero, so that all deviations are zero, a proper circumcenter exists, and

$$(\mathbf{I}-\mathbf{N})\mathbf{D}\mathbf{s}=\mathbf{0},$$

giving

$$\mathbf{D}\mathbf{s}=\frac{1}{n}(\mathbf{e}^T\mathbf{D}\mathbf{s})\mathbf{e}, \tag{6}$$

which is a form of Equation (3). When $\lambda\neq 0$ only a g-circumcenter exists. These two situations have to be considered separately, but premultiplying both (5) and (6) by $\mathbf{D}\mathbf{D}^-$ shows that $\mathbf{D}\mathbf{D}^-\mathbf{e}=\mathbf{e}$ for all real values of λ and any generalized inverse $\mathbf{D}^-$. Similarly, postmultiplying the transposes of (5) and (6) by $\mathbf{D}^-\mathbf{D}$ shows that $\mathbf{e}^T\mathbf{D}^-\mathbf{D}=\mathbf{e}^T$. The above argument requires only that $\mathbf{D}\mathbf{D}^-\mathbf{D}=\mathbf{D}$, which implies that these results must hold for any g-inverse $\mathbf{D}^-$. It is easy to verify this, for if $\mathbf{D}^=$ is any other g-inverse, then there exist matrices $\mathbf{P}$ and $\mathbf{Q}$ such that $\mathbf{D}^= = \mathbf{D}^- + (\mathbf{I}-\mathbf{D}^-\mathbf{D})\mathbf{P}+\mathbf{Q}(\mathbf{I}-\mathbf{D}\mathbf{D}^-)$, giving $\mathbf{D}\mathbf{D}^= = \mathbf{D}\mathbf{D}^- + \mathbf{D}\mathbf{Q}(\mathbf{I}-\mathbf{D}\mathbf{D}^-)$ and hence $\mathbf{D}\mathbf{D}^=\mathbf{e}=\mathbf{D}\mathbf{D}^-\mathbf{e}=\mathbf{e}$. It also follows that $\mathbf{e}^T\mathbf{D}^-\mathbf{e}$ is invariant to choice of g-inverse, a result needed below. This gives:

Theorem 2. *Any Euclidean distance matrix* $\mathbf{D}$ *with any generalized inverse* $\mathbf{D}^-$ *satisfies* $\mathbf{D}\mathbf{D}^-\mathbf{e}=\mathbf{e}$ *and* $\mathbf{e}^T\mathbf{D}^-\mathbf{D}=\mathbf{e}^T$.

This result is trivial for full-rank $\mathbf{D}$, but for other cases gives the identities that must be satisfied by distances between a set of n points. The relationship between the rank of $\mathbf{D}$ and the dimensionality of the points that generate $\mathbf{D}$ is nontrivial and is discussed in Section 3.

2.1. *Existence of a Circumcenter*

It follows from Theorem 2 that the equations (6) are always consistent with solution

$$\mathbf{s} = k\mathbf{D}^{-}\mathbf{e} + (\mathbf{I} - \mathbf{D}^{-}\mathbf{D})\mathbf{P},$$

where $\mathbf{P}$ is arbitrary and $k = (1/n)(\mathbf{e}^T\mathbf{D}\mathbf{s}) = (\mathbf{e}^T\mathbf{D}^{-}\mathbf{e})^{-1}$. Substituting for s in (3) and using Theorem 2 yields

$$R^2 = -(\mathbf{e}^T\mathbf{D}^{-}\mathbf{e})^{-1},$$

which has been shown above to be invariant to the choice of g-inverse. The only difficulty occurs when $\mathbf{e}^T\mathbf{D}^{-}\mathbf{e} = 0$, in which case R and k are infinite. In a sense this solution is acceptable, for it is a generalization of the concept of regarding three collinear points as lying on a circle of infinite radius. Nevertheless this solution is rejected in the following, and the concept of the g-circumcenter is developed.

Substituting for s into (1) yields $\mathbf{F} = \mathbf{D} - \mathbf{e}\mathbf{e}^T/\mathbf{e}^T\mathbf{D}^{-}\mathbf{e}$, which is not only invariant to the choice of g-inverse but also to $\mathbf{P}$. This establishes the uniqueness of the circumhypersphere and shows that nothing is lost by taking $\mathbf{P} = \mathbf{0}$.

THEOREM 3. *For every Euclidean distance matrix* $\mathbf{D}$, *there exists a circumhypersphere iff* $\mathbf{e}^T\mathbf{D}^{-}\mathbf{e} \neq 0$. *This has radius given by* $R^2 = -(\mathbf{e}^T\mathbf{D}^{-}\mathbf{e})^{-1}$ *corresponding to* $\mathbf{s} = \mathbf{D}^{-}\mathbf{e}/\mathbf{e}^T\mathbf{D}^{-}\mathbf{e}$.

As for Theorem 1, we have the following:

COROLLARY. *When* $\mathbf{D}$ *is Euclidean then* $\mathbf{e}^T\mathbf{D}^{-}\mathbf{e} \leqslant 0$.

2.2. *The g-Circumcenter*

When $\mathbf{e}^T\mathbf{D}^{-}\mathbf{e} = 0$, the solution to (5) is required. This equation may be written

$$\mathbf{D}^2\mathbf{s} = \lambda\mathbf{e} + \frac{1}{n}(\mathbf{e}^T\mathbf{D}\mathbf{s})\mathbf{D}\mathbf{e}. \tag{7}$$

It is now convenient to use the unique Moore-Penrose inverse $\mathbf{D}^+$ of $\mathbf{D}$. Premultiplying (7) by $\mathbf{e}^T\mathbf{D}^{+2}$ and using the commutative properties of $\mathbf{D}^+$, Theorem 2, and $\mathbf{e}^T\mathbf{D}^+\mathbf{e}=0$ gives

$$1=\mathbf{e}^T\mathbf{s}=\lambda\mathbf{e}^T\mathbf{D}^{+2}\mathbf{e},$$

identifying λ as being independent of any particular solution for s of (7). In a similar manner to that used in Section 2, any g-inverse $(\mathbf{D}^2)^-$ may be expressed in terms of $(\mathbf{D}^2)^+=\mathbf{D}^{+2}$ to show that $\mathbf{e}^T(\mathbf{D}^2)^-\mathbf{e}=\mathbf{e}^T\mathbf{D}^{+2}\mathbf{e}$ and hence that λ may be expressed in terms of any g-inverse of $\mathbf{D}^2$. This invariance does not extend to $\mathbf{e}^T(\mathbf{D}^-)^2\mathbf{e}$.

Premultiplying (7) by $\mathbf{s}^T\mathbf{D}^+$ and $\mathbf{e}^T\mathbf{D}^{+3}$ gives, respectively,

$$\mathbf{s}^T\mathbf{D}\mathbf{s}=\lambda\mathbf{s}^T\mathbf{D}^+\mathbf{e}+\frac{1}{n}(\mathbf{s}^T\mathbf{D}\mathbf{e})$$

and

$$\mathbf{e}^T\mathbf{D}^+\mathbf{s}=\lambda\mathbf{e}^T\mathbf{D}^{+3}\mathbf{e}+\frac{1}{n}(\mathbf{e}^T\mathbf{D}\mathbf{s})(\mathbf{e}^T\mathbf{D}^{+2}\mathbf{e}).$$

The squared radius of the g-circumhypersphere is the average squared distance from the g-circumcenter and is given by the average value of the elements of (2) as

$$R_g^2=\mathbf{s}^T\mathbf{D}\mathbf{s}-\frac{2}{n}\mathbf{e}^T\mathbf{D}\mathbf{s},$$

which on substituting the values found above gives

$$R_g^2=\frac{\mathbf{e}^T\mathbf{D}^{+3}\mathbf{e}}{(\mathbf{e}^T\mathbf{D}^{+2}\mathbf{e})^2},$$

showing that R_g^2 does not depend on the particular solution of (7) for s. Again $\mathbf{e}^T\mathbf{D}^{+3}\mathbf{e}$ may be written in terms of any g-inverse to give $R_g^2=\mathbf{e}^T(\mathbf{D}^3)^-\mathbf{e}/[\mathbf{e}^T(\mathbf{D}^2)^-\mathbf{e}]^2$. Expressing $(\mathbf{D}^2)^-$ in terms of $\mathbf{D}^{+2}$ and arbitrary matrices, as above, it may be verified that solutions to (7) are given by

$$\mathbf{s}=\lambda(\mathbf{D}^2)^-\mathbf{e}+\mu(\mathbf{D}^2)^-\mathbf{D}\mathbf{e}+\left[\mathbf{I}-(\mathbf{D}^2)^-\mathbf{D}^2\right]\mathbf{P}, \tag{8}$$

where $\mu = \mathbf{e}^T\mathbf{D}\mathbf{s}$ and $\mathbf{P}$ are arbitrary. Substituting (8) into (1) yields

$$\mathbf{F} = \mathbf{D} - \lambda(\mathbf{D}^{+}\mathbf{e} + \mathbf{e}^T\mathbf{D}^{+}) + \lambda^2(\mathbf{e}^T\mathbf{D}^{+3}\mathbf{e})\mathbf{e}\mathbf{e}^T$$

irrespective of the choice of g-inverse of $\mathbf{D}^2$ and of $\mathbf{P}$. This establishes the uniqueness of the g-circumcenter and also that nothing is lost by taking $\mu = 0$ and $\mathbf{P} = \mathbf{0}$.

THEOREM 4. *For any Euclidean distance matrix* $\mathbf{D}$ *with* $\mathbf{e}^T\mathbf{D}^{-}\mathbf{e} = 0$ *there exists a g-circumhypersphere given by* $\mathbf{s} = (\mathbf{D}^2)^{-}\mathbf{e}/\mathbf{e}^T(\mathbf{D}^2)^{-}\mathbf{e}$ *and with radius* R_g *where* $R_g^2 = \mathbf{e}^T(\mathbf{D}^3)^{-}\mathbf{e}/[\mathbf{e}^T(\mathbf{D}^2)^{-}\mathbf{e}]^2$.

3. RANK AND DIMENSION

DEFINITION. The dimensionality of $\mathbf{D}$ is the rank of the matrix $\mathbf{X}$ with least rank that generates $\mathbf{D}$.

Thus the dimensionality of $\mathbf{D}$ is the dimension of the space containing the points that generate $\mathbf{D}$. The requirement of *least* rank arises from the consideration that

$$\mathbf{X}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{with rank 1}$$

and

$$\mathbf{X}_2 = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{with rank 2,}$$

both generating

$$\mathbf{D} = -\frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

We shall see that the dimensionality of $\mathbf{D}$ is the same as the rank of $\mathbf{F}$, where $\mathbf{F}$ is given by (1).

Consider

$$\mathbf{F}_1 = (\mathbf{I} - \mathbf{e}\mathbf{s}^T)\mathbf{D}(\mathbf{I} - \mathbf{s}\mathbf{e}^T) \quad \text{and} \quad \mathbf{F}_2 = (\mathbf{I} - \mathbf{e}\mathbf{t}^T)\mathbf{D}(\mathbf{I} - \mathbf{t}\mathbf{e}^T),$$

where

$$\mathbf{e}^T\mathbf{s} = \mathbf{e}^T\mathbf{t} = 1.$$

We have

$$\mathbf{F}_2 = (\mathbf{I} - \mathbf{e}\mathbf{t}^T)\mathbf{F}(\mathbf{I} - \mathbf{t}\mathbf{e}^T),$$

and because $\operatorname{rank}(\mathbf{I} - \mathbf{e}\mathbf{t}^T) = n - 1$ it follows that $\operatorname{rank}(\mathbf{F}_2) \leqslant \operatorname{rank}(\mathbf{F}_1)$. Similarly $\operatorname{rank}(\mathbf{F}_1) \leqslant \operatorname{rank}(\mathbf{F}_2)$ and hence $\operatorname{rank}(\mathbf{F}_1) = \operatorname{rank}(\mathbf{F}_2)$.

Definition. A matrix of the form (1) is termed an F-matrix. A matrix of the form $\mathbf{G} = \mathbf{D} + \mathbf{g}\mathbf{e}^T + \mathbf{e}\mathbf{g}^T$ is termed a G-matrix.

The above shows that all F-matrices have the same rank. By writing $\mathbf{h} = \frac{1}{2}(\mathbf{s}^T\mathbf{D})\mathbf{e} - \mathbf{D}\mathbf{s}$ we have that $\mathbf{F} = \mathbf{D} + \mathbf{h}\mathbf{e}^T + \mathbf{e}\mathbf{h}^T$, showing that every F-matrix is a special case of a G-matrix. Also

$$\mathbf{G} = \mathbf{F} + (\mathbf{g} - \mathbf{h})\mathbf{e}^T + \mathbf{e}(\mathbf{g} - \mathbf{h})^T,$$

from which it follows that $\operatorname{rank}(\mathbf{G}) \leqslant \operatorname{rank}(\mathbf{F}) + 2$ and that $\mathbf{F} = (\mathbf{I} - \mathbf{e}\mathbf{s}^T)\mathbf{G}(\mathbf{I} - \mathbf{s}\mathbf{e}^T)$, giving $\operatorname{rank}(\mathbf{F}) \leqslant \operatorname{rank}(\mathbf{G})$. Thus

$$\operatorname{rank}(\mathbf{F}) \leqslant \operatorname{rank}(\mathbf{G}) \leqslant \operatorname{rank}(\mathbf{F}) + 2. \tag{9}$$

Suppose $\mathbf{G} = \mathbf{F} + \mathbf{m}\mathbf{e}^T + \mathbf{e}\mathbf{m}^T$ is a G-matrix of minimal rank (i.e., it has the same rank as any F-matrix). The eigenvectors of $\mathbf{m}\mathbf{e}^T + \mathbf{e}\mathbf{m}^T$ span the space determined by $\mathbf{e}$ and $\mathbf{m}$, and because these do not increase the rank of $\mathbf{F}$, they must lie in the column space of $\mathbf{F}$, i.e., there exist nonzero vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ such that

$$\mathbf{F}\mathbf{v}_1 = \mathbf{e} \quad \text{and} \quad \mathbf{F}\mathbf{v}_2 = \mathbf{m}.$$

Hence $\mathbf{G} = \mathbf{F} + \mathbf{F}\mathbf{v}_2\mathbf{v}_1^T\mathbf{F} + \mathbf{F}\mathbf{v}_1\mathbf{v}_2^T\mathbf{F}$, from which we have $(\mathbf{I} - \mathbf{e}\mathbf{s}^T)\mathbf{G}(\mathbf{I} - \mathbf{s}\mathbf{e}^T) = \mathbf{G}$. But from the definition of $\mathbf{G}$, $(\mathbf{I} - \mathbf{e}\mathbf{s}^T)\mathbf{G}(\mathbf{I} - \mathbf{s}\mathbf{e}^T) = \mathbf{F}$ and hence $\mathbf{F} = \mathbf{G}$. Thus all G-matrices of minimal rank are F-matrices.

Gower [1] showed that if $\mathbf{X}$ generates $\mathbf{D}$, then $\mathbf{X}\mathbf{X}^T$ is a G-matrix. Thus F-matrices give matrices $\mathbf{X}$ of least rank that generate $\mathbf{D}$. These results may be stated as:

Theorem 5. *All G-matrices of minimal rank are F-matrices. All F-matrices are G-matrices of minimal rank. This invariant minimal rank is the dimensionality of* $\mathbf{D}$.

It follows that the dimensionality of $\mathbf{D}$ is related to the null space of $\mathbf{F}$. Suppose $\operatorname{rank}(\mathbf{D}) = r$, so that $\mathbf{D}$ has $n - r$ linearly independent null vectors $\mathbf{x}_i (i = 1, 2, \ldots, n - r)$, where $\mathbf{D}\mathbf{x}_i = 0$. Premultiplying by $\mathbf{e}^T\mathbf{D}^-$ gives $\mathbf{e}^T\mathbf{x}_i = 0$, as was shown by a different argument in Section 1. Also

$$\mathbf{F}\mathbf{x}_i = (\mathbf{I} - \mathbf{e}\mathbf{s}^T)(\mathbf{D}\mathbf{x}_i - \mathbf{D}\mathbf{s}\mathbf{e}^T\mathbf{x}_i) = \mathbf{0}.$$

Thus the null vectors of $\mathbf{D}$ are also null vectors of $\mathbf{F}$, but $\mathbf{F}$ will also have other null vectors, of which $\mathbf{s}$ is clearly one—the condition $\mathbf{s}^T\mathbf{e} = 1$ ensures that $\mathbf{s}$ is linearly independent of all the $\mathbf{x}_i$. Suppose $\mathbf{y}$ is any other null vector of $\mathbf{F}$; then

$$\mathbf{D}\mathbf{y} = k\mathbf{e} + (\mathbf{e}^T\mathbf{y})\mathbf{D}\mathbf{s}, \tag{10}$$

where

$$k = \mathbf{s}^T\mathbf{D}\mathbf{y} - (\mathbf{s}^T\mathbf{D}\mathbf{s})(\mathbf{e}^T\mathbf{y}).$$

Premultiplying both sides by $\mathbf{e}^T\mathbf{D}^-$ shows that either $k = 0$ or $\mathbf{e}^T\mathbf{D}^-\mathbf{e} = 0$. In the first case (10) becomes

$$\mathbf{D}(\mathbf{y} - (\mathbf{e}^T\mathbf{y})\mathbf{s}) = 0,$$

so that $\mathbf{y} - (\mathbf{e}^T\mathbf{y})\mathbf{s} = \sum_{i=1}^{n-r}\lambda_i\mathbf{x}_i$ for some λ_i $(i = 1, 2, \ldots, n - r)$, showing that $\mathbf{y}$ is linearly dependent on the already established null vectors of $\mathbf{F}$. The rank of $\mathbf{F}$ is therefore $r - 1$.

When $\mathbf{e}^T\mathbf{D}^-\mathbf{e} = 0$, (10) gives

$$\mathbf{D}(\mathbf{y} - (\mathbf{e}^T\mathbf{y})\mathbf{s}) = k\mathbf{e},$$

or

$$\mathbf{D}(\mathbf{y} - (\mathbf{e}^T\mathbf{y})\mathbf{s} - k\mathbf{D}^-\mathbf{e}) = \mathbf{0},$$

giving

$$\mathbf{y} = (\mathbf{e}^T\mathbf{y})\mathbf{s} + \sum_{i=1}^{n-1}\lambda_i\mathbf{x}_i + k\mathbf{D}^-\mathbf{e}. \tag{11}$$

Thus the only null vector of $\mathbf{F}$ that may be linearly independent of the $\mathbf{x}_i$ and s is $\mathbf{D}^-\mathbf{e}$. The condition for dependence is that there exist α_i and α, not all zero, such that

$$\mathbf{D}^-\mathbf{e} = \sum_{i=1}^{n-r} \alpha_i \mathbf{x}_i + \alpha \mathbf{s}.$$

Premultiplying respectively by $\mathbf{e}^T$ and $\mathbf{D}$ using Theorem 2 gives

$$\alpha = \mathbf{e}^T\mathbf{D}^-\mathbf{e} \quad \text{and} \quad \mathbf{e} = \alpha\mathbf{D}\mathbf{s},$$

so that when $\mathbf{e}^T\mathbf{D}^-\mathbf{e} = 0$ we have a contradiction and linear dependence is not possible; $\mathbf{D}^-\mathbf{e}$ is then a further independent null vector of $\mathbf{F}$. It must be established that different choices of g-inverse do not give additional independent null vectors. Expressing $\mathbf{D}^-$ in terms of the Moore-Penrose inverse $\mathbf{D}^+$ and matrices $\mathbf{P}$ and $\mathbf{Q}$ gives $\mathbf{D}^- = \mathbf{D}^+ + (\mathbf{I} - \mathbf{D}^+\mathbf{D})\mathbf{P} + \mathbf{Q}(\mathbf{I} - \mathbf{D}\mathbf{D}^+)$. Hence from Theorem 2, $\mathbf{D}^-\mathbf{e} = \mathbf{D}^+\mathbf{e} + (\mathbf{I} - \mathbf{D}^+\mathbf{D})\mathbf{p}$ where $\mathbf{p} = \mathbf{P}\mathbf{e}$. Now $\mathbf{I} - \mathbf{D}^+\mathbf{D} = \sum_{i=1}^{r}\mathbf{x}_i\mathbf{x}_i^T$ so that $\mathbf{D}^-\mathbf{e} = \mathbf{D}^+\mathbf{e} + \sum_{i=1}^{r} l_i\mathbf{x}_i$, where $l_i = \mathbf{x}_i^T\mathbf{p}$. It follows that the null vectors $\mathbf{x}_i$ of $\mathbf{D}$, together with s and $\mathbf{D}^-\mathbf{e}$ (for any g-inverse $\mathbf{D}^-$), span the null space of $\mathbf{F}$, which therefore must have rank $r - 2$. These results, with Theorems 3 and 4, may be combined to give:

THEOREM 6. *All the null vectors of* $\mathbf{D}$ *are also null vectors of* $\mathbf{F}$, *and they satisfy* $\mathbf{e}^T\mathbf{x}_i = 0$. $\mathbf{F}$ *always has* s *as a further null vector. If rank*$(\mathbf{D}) = r$ *then the dimensionality of* $\mathbf{D}$ *is*:

(i) $r - 1$ *iff* $\mathbf{e}^T\mathbf{D}^-\mathbf{e} \neq 0$, *in which case the generating points lie on the surface of a hypersphere, or*

(ii) $r - 2$ *iff* $\mathbf{e}^T\mathbf{D}^-\mathbf{e} = 0$, *in which case the generating points cannot lie on the surface of a hypersphere and* $\mathbf{D}^-\mathbf{e}$ *is a further independent null vector of* $\mathbf{F}$.

4. NON-EUCLIDEAN DISTANCE

When $\mathbf{D}$ is non-Euclidean, $\mathbf{F}$ is not p.s.d. and no real $\mathbf{X}$ can generate $\mathbf{D}$. For those $\mathbf{D}$ for which $\mathbf{D}\mathbf{D}^-\mathbf{e} = \mathbf{e}$ remains true, the results found in previous sections remain valid. However, when $\mathbf{D}\mathbf{D}^-\mathbf{e} \neq \mathbf{e}$, the equations (5) are not consistent and neither a circumcenter nor a g-circumcenter exists. The quantity $\mathbf{s}^T\mathbf{D}(\mathbf{I} - \mathbf{N})\mathbf{D}\mathbf{s}$ may then be made arbitrarily close to zero. Theorem 5 still gives the dimensionality of $\mathbf{D}$, but the nonreal nature of $\mathbf{X}$ needs analysis for a full understanding of its structure. We shall see that $\mathbf{X}$ derived from any F-matrix will have r real and s purely imaginary columns and that r and s are invariant. Further, for any G-matrix the corresponding values will not be less than r and s.

4.1. *Rank and Dimension — Non-Euclidean Case*

Although Theorem 5 still gives the dimensionality of $\mathbf{D}$ as the rank of $\mathbf{F}$, when $\mathbf{DD}^{-}\mathbf{e} \neq \mathbf{e}$ the rank of $\mathbf{F}$ will now equal r, the rank of $\mathbf{D}$. This essential difference from the Euclidean case is established as follows.

When $\mathbf{DD}^{-}\mathbf{e} \neq \mathbf{e}$, then $\mathbf{D}$ must be singular. Suppose $\mathbf{D}$ has nonnull vectors $\mathbf{x}_i$ $(i = 1,2,\ldots,r)$ and null vectors $\mathbf{x}_i$ $(i = r+1, r+2,\ldots,n)$ chosen to be orthonormal. Then $\mathbf{DD}^{+} = \mathbf{x}_1\mathbf{x}_1^T + \mathbf{x}_2\mathbf{x}_2^T + \cdots + \mathbf{x}_i\mathbf{x}_i^T$ and $\sum_{i=1}^{n}\mathbf{x}_i\mathbf{x}_i^T = \mathbf{I}$. Thus

$$\mathbf{DD}^{+}\mathbf{e} = \mathbf{e} - \sum_{i=r+1}^{n} \mathbf{x}_i\mathbf{x}_i^T\mathbf{e}.$$

Now $\mathbf{DD}^{-}\mathbf{e} \neq \mathbf{e}$ implies $\mathbf{DD}^{+}\mathbf{e} \neq \mathbf{e}$, so that $\sum_{i=r+1}^{n}\mathbf{x}_i(\mathbf{x}_i^T\mathbf{e}) \neq \mathbf{0}$ and for at least one null vector $\mathbf{x}$ of $\mathbf{D}$ we must have $\mathbf{x}^T\mathbf{e} \neq 0$. This differs from the Euclidean case, because we may now choose $\mathbf{s} = \mathbf{x}$ so that $\mathbf{s}^T\mathbf{e} = 1$ but $\mathbf{Ds} = \mathbf{0}$. The corresponding F-matrix becomes

$$\mathbf{F} = (\mathbf{I} - \mathbf{es}^T)\mathbf{D}(\mathbf{I} - \mathbf{se}^T) = \mathbf{D}.$$

The proof of Theorem 5 that rank($\mathbf{F}$) is minimal and invariant to the choice of $\mathbf{s}$ such that $\mathbf{s}^T\mathbf{e} = 1$ remains valid, so that when $\mathbf{DD}^{-}\mathbf{e} \neq \mathbf{e}$ the dimensionality of $\mathbf{D}$ is its rank.

This gives the following:

THEOREM 7. *When* $\mathbf{D}$ *is non-Euclidean, either*

(i) $\mathbf{DD}^{-}\mathbf{e} = \mathbf{e}$ *and the dimensionality of* $\mathbf{D}$ *is given by Theorems* 5 *and* 6, *or*

(ii) $\mathbf{DD}^{-}\mathbf{e} \neq \mathbf{e}$ *and the dimensionality of* $\mathbf{D}$ *is its rank.*

4.2. *Real and Imaginary Dimensions*

The above has shown that dimensionality is well defined in the non-Euclidean case but has not established how the dimensions are allocated between real and imaginary components. To investigate this is the purpose of this section.

Any symmetric matrix $\mathbf{A}$ of rank $r+s$ may be written $\mathbf{A} = \mathbf{LSL}^T$, where $\mathbf{L}$ has $r+s$ columns and is of rank $r+s$, and $\mathbf{S}$ is a diagonal matrix of signs with r positive and s negative units. Such decompositions are not unique, but the fundamental result on signature is that the values of r and s are invariant over all such decompositions; the invariant quantity $r - s$ is termed the signature. Suppose $\mathbf{U}$ is any matrix such that $\mathrm{rank}(\mathbf{UAU}^T) = \mathrm{rank}(\mathbf{A})$. Then $\mathbf{UAU}^T = (\mathbf{UL})\mathbf{S}(\mathbf{UL})^T$, and since this has the same rank as $\mathbf{A}$, then $\mathrm{rank}(\mathbf{UL}) = \mathrm{rank}(\mathbf{L})$. It follows that $\mathbf{A}$ and $\mathbf{UAU}^T$ have the same signature, because they share the same $\mathbf{S}$. Any pair of F-matrices (which have already been shown to have equal rank) are related by

$$\mathbf{F}_1 = \left(\mathbf{I} - \mathbf{e}\mathbf{s}_1^T\right)\mathbf{D}\left(\mathbf{I} - \mathbf{s}_1\mathbf{e}^T\right) = \left(\mathbf{I} - \mathbf{e}\mathbf{s}_1^T\right)\mathbf{F}_2\left(\mathbf{I} - \mathbf{s}_1\mathbf{e}^T\right),$$

and setting $\mathbf{U} = \mathbf{I} - \mathbf{e}\mathbf{s}^T$ shows that $\mathbf{F}_1$ and $\mathbf{F}_2$, and hence all F-matrices, have the same signature.

Putting $\mathbf{F} = \mathbf{LSL}^T$, where $\mathbf{L} = (\mathbf{l}_1, \mathbf{l}_2, \ldots, \mathbf{l}_{r+s})$, we may expand the quadratic form $\mathbf{x}^T\mathbf{F}\mathbf{x}$ to give

$$\mathbf{x}^T\mathbf{F}\mathbf{x} = \sum_{p=1}^{r} \left(\mathbf{l}_p^T\mathbf{x}\right)^2 - \sum_{p=r+1}^{r+s} \left(\mathbf{l}_p^T\mathbf{x}\right)^2,$$

and setting $x_i = 1$, $x_j = -1$, and $x_k = 0$ $(k \neq i, j)$ gives

$$f_{ii} + f_{jj} - 2f_{ij} = d_{ij}^2 = \sum_{p=1}^{r} \left(l_{pi} - l_{pj}\right)^2 - \sum_{p=r+1}^{r+s} \left(l_{pi} - l_{pj}\right)^2.$$

This is the usual "Pythagorean" representation of squared distance in terms of coordinates l_{pi} $(p = 1, 2, \ldots, r + s)$, except that for $p > r$ the coordinates become purely imaginary. This has shown:

THEOREM 8. *When* $\mathbf{D}$ *is non-Euclidean, its dimensionality* $r + s$*, obtained from any F-matrix, is derived from a generating matrix of coordinates in r real and s imaginary dimensions. The values of r and s are invariant in all F-matrices and hence in all least-rank representations.*

4.3. *Minimality Properties of Real and Imaginary Components of Dimension*

Theorem 8 permits one to think in a well-defined manner of dimensionality associated with non-Euclidean distance matrices. We shall write this dimensionality as $F(r, s)$. Although no F-matrix can generate a lower value of r or of s, representations derived from higher ranking G-matrices, which must be consistent with (9), might; e.g., it remains to be shown that $G(r - 1, s + 2)$

is impossible. A detailed examination of all possible coordinate representations derived from G-matrices other than F-matrices is therefore needed. To do this requires an analysis of the relationships between the eigenvalues of an F-matrix and of a G-matrix; the numbers of positive and negative eigenvalues, of course, give the values of r and s in the coordinate representations. Thus we wish to relate the eigenvalues $(\gamma_1, \gamma_2, \ldots, \gamma_n)$ of $\mathbf{G}$ to the eigenvalues $(\phi_1, \phi_2, \ldots, \phi_n)$ of $\mathbf{F}$, where it is assumed that $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_n$ and $\phi_1 \geqslant \phi_2 \geqslant \cdots \geqslant \phi_n$. We have that $\mathbf{G} = \mathbf{F} + \mathbf{h}e^T + e\mathbf{h}^T$.

The eigenvalues of the rank-2 matrix $\mathbf{H} = \mathbf{h}\mathbf{e}^T + \mathbf{e}\mathbf{h}^T$ are

$$h_1 = \mathbf{e}^T\mathbf{h} + \left[n(\mathbf{h}^T\mathbf{h})\right]^{1/2} \geqslant 0$$

and

$$h_n = \mathbf{e}^T\mathbf{h} - \left[n(\mathbf{h}^T\mathbf{h})\right]^{1/2} \leqslant 0$$

together with $h_2 = h_3 = \cdots = h_{n-1} = 0$. Now the relationship between the eigenvalues of $\mathbf{G}$, $\mathbf{F}$, and $\mathbf{H}$ is given by the minimax theorem (see [6, p. 101]) as

$$\gamma_{p+q-1} \leqslant \phi_p + h_q. \tag{12}$$

Also writing $\mathbf{F} = \mathbf{G} + (-\mathbf{H})$ gives

$$\phi_{p+q-1} \leqslant \gamma_p - h_{n-q+1},$$

i.e.,

$$\gamma_p \geqslant \phi_{p+q-1} + h_{n-q+1}. \tag{13}$$

Substituting the values indicated below for p and q in (12) and (13) gives:

p	q	From (12)	From (13)
1	1	$\gamma_1 \leqslant \phi_1 + h_1$	$\gamma_1 \geqslant \phi_1 + h_n$
1	2	$\gamma_2 \leqslant \phi_1$	$\gamma_1 \geqslant \phi_2$
2	2	$\gamma_3 \leqslant \phi_2$	$\gamma_2 \geqslant \phi_3$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$n-1$	2	$\gamma_n \leqslant \phi_{n-1}$	$\gamma_{n-1} \geqslant \phi_n$

The interleaving of these eigenvalues is best illustrated diagrammatically as in

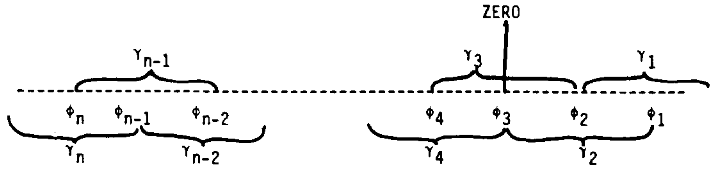

FIG. 1. The interleaving of the eigenvalues of **G** and **F** when n is even. The case n odd is essentially the same, but the values of $\gamma_n, \gamma_{n-2}, \ldots$ then occur above the line and those for $\gamma_{n-1}, \gamma_{n-3}, \ldots$ occur below the line.

Figure 1, where the fact that **F** has at least one zero eigenvalue has been indicated by showing ϕ_3 as zero.

From Figure 1 it is clear that **G** has one more nonzero eigenvalue than does **F**, and that when $F(r, s)$ gives the number of positive and negative eigenvalues of **F**, then the corresponding values for **G** are either $G(r+1, s)$ or $G(r, s+1)$, depending on whether γ_3 is positive or negative. The possibility that rank(**G**) = rank(**F**)+2 has already been mentioned. This can occur only when **F** has two or more zero eigenvalues. The interleaving is then given by Figure 2. **G** may now have one more positive and one more negative eigenvalue than does **F**, giving $G(r+1, s+1)$. These results may be stated as

THEOREM 9. *If* **D** *is a distance matrix, possibly non-Euclidean, that is associated with the form* $F(r, s)$, *then coordinate representations that generate* **D** *may be derived from* $F(r, s)$ *itself or from* $G(r+1, s)$, $G(r, s+1)$ *or, when* $r + s \leqslant n - 2$, *from* $G(r+1, s+1)$.

Note that this shows that not only do the forms $F(r, s)$ have minimal rank, but also they have minimal values of both r and s. Thus coordinates derived from F-matrices are the only ones whose ranks are the dimensionality of **D**.

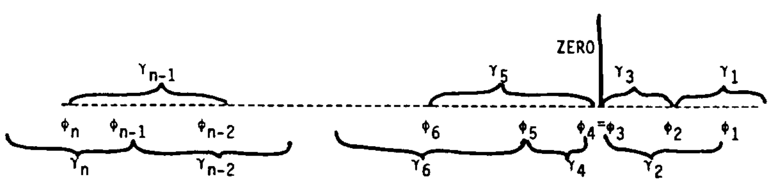

FIG. 2. The interleaving of the eigenvalues of **G** and **F** for multiple zero eigenvalues of **F**.

4.4. *Illustration of the Four Forms of Full-Rank Representation of a Distance-matrix*

These results may be illustrated using the matrix

$$\mathbf{D} = -\frac{1}{2}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix},$$

which represents two coincident points at unit distance from a third point. Setting $\mathbf{s} = \mathbf{e}_1$ yields an F-matrix $\mathbf{F} = \mathbf{e}_1^T\mathbf{e}_1$ giving the minimal dimension coordinate representation with $r = 1$ and $s = 0$:

$$F(1,0) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The rank-2 real representation is typified by

$$G(2,0) = \begin{pmatrix} 0 & 1 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}$$

or any plane rotation of it. Setting $\mathbf{g} = \mathbf{0}$ and hence $\mathbf{G} = \mathbf{D}$ gives

$$G(1,1) = \begin{pmatrix} 2^{-5/4} & i2^{-5/4} \\ 2^{-5/4} & i2^{-5/4} \\ 2^{-3/4} & -i2^{-3/4} \end{pmatrix},$$

while setting $\mathbf{g} = (\frac{1}{2}, 1, \frac{1}{2})^T$ gives

$$G(2,1) = \begin{pmatrix} 0.30917 & 0.22014 & i1.06960 \\ 0.33527 & -0.17307 & i1.46368 \\ -0.67940 & 0.01477 & i1.20904 \end{pmatrix},$$

In the last two examples spectral decompositions of $\mathbf{G}$ have been used, though any other decomposition would suffice to give results of the same forms.

All four sets of coordinates generate the same distance matrix $\mathbf{D}$, although their ranks and signatures differ. This illustration has represented a Euclidean matrix; if $\mathbf{D}$ is non-Euclidean, the same four types of representation occur but with imaginary columns in every case.

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