Discussion of a Set of Points in Terms of Their Mutual Distances*

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Abstract

Necessary and sufficient conditions are given for a set of numbers to be the mutual distances of a set real points in Euclidean space, and matrices are found whose ranks determine the dimension of the smallest Euclidean space containing such points. Methods are indicated for determining the configuration of these points, and for approximating to them by points in a space of lower dimensionality.

Ordinarily a set of points is specified by giving its coordinates in a suitable reference system; and the dimensionality of the set, the problem of approximating it by a lower dimensional set, etc., can be discussed in terms of these coordinates. It may be, however, that only the distances of the points from each other are known, and it is desired to give a similar discussion on this basis.

Consider a set of n points, and let $a_i = 1 \ \ldots \ n-1$, be the vector from point n to point i. Let a_{ij} be the component of a_i along the j-th axis of an orthogonal coordinate system with origin at point n and let A denote the matrix (a_{ij}). The dimensionality of the point set is equal to the rank of A and to the rank of $B = AA'$. The elements of B are given by $b_{ij} = a_i.a_j$. The vector from point i to point j is $v_{ij} = a_j - a_i$, and by taking the scalar product of each side with itself there results the familiar 'cosine law':

$$d^2{}_{ij} = d^2{}_{jn} + d^2{}_{in} - 2\, a_i \cdot a_j \,,$$

where d_{ij} is the distance between points i and j. From this it follows at once that

$$b_{ij} = (d^2_{in} + d^2_{jn} - d^2_{ij})/2 \,, \tag{1}$$

so that AA' is expressible in terms of the mutual distances only. Thus

(I) The dimensionality of a set of points with mutual distances d_{ij} is equal to the rank of the $n-1$ square matrix B whose elements are defined by (1).

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A matrix first given by Cayley in 1841, and involving the points in more symmetric fashion, may be used in place of the matrix B. First, the matrix $C = -2B$ has evidently the same rank r as B. Border this to obtain the $\eta + 1$ square matrix

$$D = \left\{ \begin{array}{ccc} C & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{array} \right\}.$$

Since C is symmetric it has a non-vanishing $r \times r$ principal minor M_r. The determinant of the minor

$$S = \left\{ \begin{array}{ccc} M_r & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{array} \right\}$$

has for its value

$$|s| = |M_r| \cdot \left| \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right| = -|M_r|,$$

as we see by a Laplace expansion. Hence the matrix D has rank $r + 2$ at least. If D had a greater rank there would be some minor M_{r+1} of order $r + 1$ of C for which

$$\left\{ \begin{array}{ccc} M_{r+1} & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{array} \right\}$$

is non-singular. But since M_{r+1} is singular, the determinant of this matrix is $-|M_{r+1}| = 0$. Hence the rank of D is exactly $r + 2$.

Now perform the following operations on D:

These are so-called elementary transformations, and do not change the rank of a matrix. The result is

$$F = \left\{ \begin{array}{ccccc} 0 & d_{12}^2 & \dots & d_{1n}^2 & 1 \\ d_{21}^2 & 0 & \dots & d_{2n}^2 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ d_{n1}^2 & d_{n2}^2 & \dots & 0 & 1 \\ 1 & 1 & \dots & 1 & 0 \end{array} \right\} \qquad (2)$$

Thus

(II) The dimensionality of a set of points with mutual distances d_{ij} is less than the rank of the $n + 1$ square matrix F given by (2).

Consider next the conditions under which a set of numbers $d_{ij} = d_{ji}$ can be the mutual distances of a set of real points in Euclidean space. It is evident to begin with that if such a set of points exists then any other such set defines a figure which is congruent (or symmentric) to the first. Moreover, if we form the matrix B whose elements are defined by Equation (1), then necessarily B is symmetric, and is equal to the product AA' of the matrix A of coordinates of these points, in any coordinate system with origin at point n, by the transpose of this matrix. Hence B is positive semi-definite.

Conversely, if B is positive semi-definite, then such points do exist, and to show this we need only exhibit a matrix A. Since B then has only positive or zero latent roots, there exists an orthogonal matrix σ such that

$$B = \sigma\, L^2\, \sigma' = (\sigma L)(\sigma L)', \tag{3}$$

where

$$L^2 = [\lambda_1^2, \lambda_2^2 \ldots \lambda_r^2, 0 \ldots 0] \tag{4}$$

is a diagonal matrix of the latent roots of B. Hence we may take

$$A = \sigma\, L, \tag{5}$$

and the theorem is proved:

(III) *A necessary and sufficient condition for a set of numbers* $d_{ij} = d_{ji}$ *to be the mutual distances of a real set of points in Euclidean space is that the matrix* B *whose elements are defined by equation* (1) *be positive semi-definite; and in this case the set of points is unique apart from a Euclidean transformation.*

For the case $n = 3$, the condition that B be positive semi-definite is equivalent to the familiar triangle law: that each side of a triangle be less than, or equal to, the sum of the other two. In general, the positiveness of the determinant of the 2×2 principal minor on rows i and j gives the triangle relation on d_{in}, d_{jn} and d_{ij}; while the corresponding requirement on the larger principal minors gives an extension of this law. The present problem of determining a matrix A which specifies the configuration of the set of points is merely a generalization of the familiar trigonometry problem of finding a triangle when the lengths of its sides are given.

For the actual factorization of the matrix B we may refer to a method given by Thurstone*. Methods of fitting a lower dimensional set of points to a given set are also available†, so that the complete analysis of a set of points is possible given the mutual distances only.

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*Thurstone, L. L., *Vectors of Mind*, Chicago: University of Chicago Press, p. 78

†Eckart, Carl, and Young, Gale, "The Approximation of One Matrix by Another of Lower Rank," *Psychometrika*, 1936, **1**, 211-218.