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Euclidean Distance Geometry

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Abstract

A unified account is given of distance matrices in the Euclidean geometry of many points in many dimensions. The aim is to make some interesting and useful results accessible to applied scientists, including statisticians.

1. Introduction

Everyone is familiar with properties of triangles expressed in terms of their angles and the lengths of their sides. Yet corresponding results for n points in multidimensional Euclidean space are not well known. One reason for this seems to be that triangles are studied by the coordinate-free methods of classical geometry, whereas the properties of n points are usually explored through the linear algebra associated with coordinate geometry, an approach that does not lend itself naturally to handling distances. Of course mathematicians have studied distance geometries in depth and a rigorous account of their work is given by Blumenthal (1970). Such work is of a very general nature and is not easily accessible to non-specialists. In any case Euclidean distance is only one type of distance and, although an important one, it does not receive prominence in general theoretical presentations.

Despite the development of numerous types of geometry, Euclidean geometry is still by far the most used geometrical tool of applied scientists. For example, statisticians find it useful to regard samples, on each of which p observations have been made, as a set of points in a p-dimensional Euclidean space. They then examine selected cross-sections of this space, or seek representations in fewer dimensions that give some acceptable degree of approximation to the distances in the full space.

In the following an elementary account is given of some of the basic properties of points $P_1, P_2, \ldots, P_n$ of a Euclidean space where the distance d_{ij} between P_i and P_j is Euclidean. For $n = 3$ these distances are the lengths of the sides of a triangle $P_1P_2P_3$. So far as possible a coordinate-free approach is adopted and many of the results given below will be expressed in terms of the distances.

The distances may be collected into a symmetric matrix with d_{ij} as the element in the (i, j)th position and with zero diagonal. Such a matrix might be termed a distance matrix but it turns out to be more convenient to work in terms of the matrix $\boldsymbol{D} = (-\frac{1}{2}d_{ij}^2)$ and I shall refer to this as a distance matrix. Some of the results given below are valid only for non-degenerate sets of n points, i.e. points that lie in exactly

$n-1$ dimensions. Such results are easily recognised for they involve the inverse of the matrix $\boldsymbol{D}$ and $\boldsymbol{D}$ is singular for degenerate systems.

Symmetric matrices that have non-negative elements and zero diagonal values arise as data in many experimental sciences. Whether or not their values may be regarded as distances between points in a Euclidean space is a matter that deserves investigation. Even when $\boldsymbol{D}$ is not Euclidean, there may be a matrix $\boldsymbol{D}^*$ which is Euclidean and whose elements differ little from those of $\boldsymbol{D}$. Thus we can ask what is the best Euclidean approximation to a non-Euclidean matrix $\boldsymbol{D}$. The investigation of such problems has motivated my interest in Euclidean distance geometry. Although several of the results given below are well known, others I have been unable to find in the literature. Nevertheless, I doubt whether there is much new in the following. A connected account of the subject, if available, is hard to find and I hope that this one will be of general interest, and a useful reference for other workers.

2. When is a distance matrix Euclidean

All distances are metrics, that is they satisfy the 'triangle law' $d_{ij} \leq d_{ik} + d_{jk}$ for all i, j, k. When d_{12} exceeds d_{13} and d_{23} the condition $d_{12} \leq d_{13} + d_{23}$ is a necessary and sufficient condition for a triangle to have a Euclidean representation. We shall say that a Euclidean triangle is *closed*. With four points the position is more complicated. Figure 1 illustrates four points for which all four triangles are closed, but clearly without a Euclidean representation. Although it is necessary for all triangles to be closed, this is not sufficient to guarantee a Euclidean representation. This suggests that the conditions for a set of distances to be Euclidean are more subtle than might be at first thought.

A simple approach is to attempt to construct a set of real coordinates that reproduce the distances. It is always possible to put the first point at the origin and the second, distance d_{12} from the origin on the first coordinate axis. Thereafter there are difficulties when $\boldsymbol{D}$ is non-Euclidean. However, when $\boldsymbol{D}$ is Euclidean the third point may be put in the plane of the first two axes, the fourth point in the space of the first three axes and so

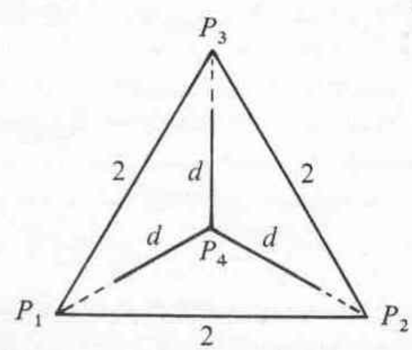

Fig. 1. This configuration is not Euclidean when $1 < d < 2/\sqrt{3}$ because setting P_4 at the centroid gives the only two-dimensional configuration for which $P_4P_1 = P_4P_2 = P_4P_3 = d$ and this requires $d = 2/\sqrt{3}$. Other Euclidean configurations exist in three dimensions, but these require $d > 2/\sqrt{3}$. Nevertheless, all the triangles are closed.

on. In this way a matrix $\boldsymbol{X}$ is built up, whose rows give the coordinates of the points. $\boldsymbol{X}$ is 0 on and above the principal diagonal and hence has the triangular form

$$\boldsymbol{X} = \begin{bmatrix} 0 & & & & & & \\ d_{21} & 0 & & & & & \\ x_{31} & x_{32} & 0 & & & & \\ \cdot & \cdot & \cdot & \cdot & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \\ x_{n1} & x_{n2} & x_{n3} & \cdot & \cdot & x_{n,n-1} & 0 \end{bmatrix}.$$

Clearly $\boldsymbol{D}$ is Euclidean if and only if $\boldsymbol{X}$ is real. This statement is almost tautological and needs strengthening to be of value. Gower (1968) gives specific formulae for adding an rth row to $\boldsymbol{X}$, given the first $r-1$ rows and the first r elements of the rth row of $\boldsymbol{D}$. When $P_1, P_2, \ldots, P_{r-1}$ have real coordinates (i.e. are Euclidean) these formulae give real coordinate values for $(x_{r1}, x_{r2}, \ldots, x_{r,r-2})$. The coordinate $x_{r,r-1}$ in the new dimension added is obtained as the square root of a real quantity. Therefore when $x_{r,r-1}^2 \geq 0$ the configuration remains Euclidean and when $x_{r,r-1}^2 < 0$ there is no Euclidean representation of the first r points. Thus we have the following theorem.

Theorem 1. $\boldsymbol{D}$ is Euclidean iff no principal sub-diagonal value of $\boldsymbol{X}$ is purely imaginary.

Another way of putting this result is that when $\boldsymbol{D}$ is non-Euclidean at least one principal sub-diagonal value of $\boldsymbol{X}$ is purely imaginary.

This theorem immediately leads to some well-known results based on the concept of content, the multidimensional analogue of volume. Some discussion of content is given below in Section 4 and if the coordinates $\boldsymbol{X}$ are substituted in the definition of content C_n given there, it will be found that the content of the first r points is given by

$$(r-1)!C_r = \prod_{i=2}^{r} x_{i,i-1}.$$

It is then evident that when the points $P_1, P_2, \ldots, P_r$ have a real Euclidean representation then their squared content must be positive. The converse that positive squared content implies a Euclidean configuration is not true, for an even number of terms in the product may be purely imaginary. However when the squared content of $P_1, P_2, \ldots, P_r$ is positive for $r = 2, 3, \ldots, n$, this is sufficient, as well as necessary, for $\boldsymbol{D}$ to be Euclidean. Details of this, and allied, results can be found in Blumenthal (1970), p. 100. Note that the use of content may fail when $\boldsymbol{D}$ is degenerate. For then $C_r = 0$ for some r and $C_s = 0$ for all $s \geq r$. The matrix $\boldsymbol{X}$, however, will still exhibit any non-Euclideanarity by containing imaginary values, though not necessarily on the principal sub-diagonal. The results based on content are rather cumbersome in practical use and are not fruitful in deriving further properties.

An alternative approach. A different approach is based directly on the fundamental property of Euclidean space; that distance is expressed by Pythagoras's theorem. Thus if $\boldsymbol{D}$ is Euclidean there exists a matrix of coordinates ${}_n\boldsymbol{X}_r$ (from which we derive $\boldsymbol{E} = \boldsymbol{X}\boldsymbol{X}'$) such that $d_{ij}^2 = e_{ii} + e_{jj} - 2e_{ij}$ which is Pythagoras's theorem in light disguise. Suppose $\boldsymbol{Y}$ and $\boldsymbol{F}$ $(= \boldsymbol{Y}\boldsymbol{Y}')$ are other matrices with this property, then without loss of generality we can write $\boldsymbol{F} = \boldsymbol{D} + \boldsymbol{G}$ so that $d_{ij}^2 = f_{ii} + f_{jj} - 2f_{ij} = d_{ij}^2 + g_{ii} + g_{jj} - 2g_{ij}$. Hence $g_{ij} = \frac{1}{2}(g_{ii} + g_{jj})$ or $\boldsymbol{G} = \boldsymbol{g}\boldsymbol{1}' + \boldsymbol{1}\boldsymbol{g}'$ where $g_i = \frac{1}{2}g_{ii}$ and $\boldsymbol{1}$ is a vector of units. This shows that all symmetric matrices $\boldsymbol{F}$ with decomposition $\boldsymbol{Y}\boldsymbol{Y}'$, where the rows of $\boldsymbol{Y}$ are coordinates that generate the squared distances d_{ij}^2, have the form

$$\boldsymbol{F} = \boldsymbol{D} + \boldsymbol{g}\boldsymbol{1}' + \boldsymbol{1}\boldsymbol{g}'. \tag{1}$$

The above is a fundamental result showing that we have to consider only matrices that depart from $\boldsymbol{D}$ by the special form $\boldsymbol{g}\boldsymbol{1}' + \boldsymbol{1}\boldsymbol{g}'$, which has rank 2. Clearly if $\boldsymbol{Y}$ is to be real, $\boldsymbol{F}$ must be positive semi-definite (p.s.d.). Thus when $\boldsymbol{D}$ is Euclidean, it must be possible to choose a vector $\boldsymbol{g}$ so that $\boldsymbol{F}$ is p.s.d. The choice of $\boldsymbol{g}$ will not be unique but all choices will generate the same distances, so that the resulting coordinates $\boldsymbol{Y}$ will represent solutions with different translations of origin and different orthogonal rotations of the axes. There is also the possibility that different settings of $\boldsymbol{g}$ will generate $\boldsymbol{F}$ and hence $\boldsymbol{Y}$ with ranks that differ (by at most 1). For example the coordinates $\boldsymbol{Y}_2 = \begin{bmatrix} 1 & 1 \\ 1 & 3 \end{bmatrix}$ have rank 2 but are one-dimensional and could be represented by the rank-1 matrix $\boldsymbol{Y}_1 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$ involving only a change of origin. Solutions $\boldsymbol{Y}$ differing only by a translation, will be said to be *equivalent*.

It is possible to choose $\boldsymbol{g}$ so that $\boldsymbol{F}$ has least rank, but it is better to investigate the possibilities of expressing $\boldsymbol{F}$ in the mulitiplicative form

$$\boldsymbol{F} = (\boldsymbol{I} - \boldsymbol{1}\boldsymbol{s}')\boldsymbol{D}(\boldsymbol{I} - \boldsymbol{s}\boldsymbol{1}'). \tag{2}$$

If for every $\boldsymbol{g}$ we can find an $\boldsymbol{s}$, then the forms (1) and (2) are alternative expressions for the same thing.

We have seen that equivalent settings of $\boldsymbol{Y}$ correspond to different translations $\boldsymbol{m}$ (say) giving new coordinates $\boldsymbol{Y} + \boldsymbol{1}\boldsymbol{m}'$. Let us choose $\boldsymbol{m} = -\boldsymbol{Y}'\boldsymbol{s}$ where $\boldsymbol{s}'\boldsymbol{g} = 0$ and $\boldsymbol{s}'\boldsymbol{1} = 1$ then $(\boldsymbol{Y} + \boldsymbol{1}\boldsymbol{m}') = (\boldsymbol{I} - \boldsymbol{1}\boldsymbol{s}')\boldsymbol{Y}$ and corresponding to $\boldsymbol{F}$ we have

$$\begin{aligned} \boldsymbol{F}^* = (\boldsymbol{I} - \boldsymbol{1}\boldsymbol{s}')\boldsymbol{Y}\boldsymbol{Y}'(\boldsymbol{I} - \boldsymbol{1}\boldsymbol{s}') &= (\boldsymbol{I} - \boldsymbol{1}\boldsymbol{s}')(\boldsymbol{D} + \boldsymbol{1}\boldsymbol{g}' + \boldsymbol{g}\boldsymbol{1}')(\boldsymbol{I} - \boldsymbol{s}\boldsymbol{1}') \\ &= (\boldsymbol{I} - \boldsymbol{1}\boldsymbol{s}')\boldsymbol{D}(\boldsymbol{I} - \boldsymbol{s}\boldsymbol{1}'). \end{aligned}$$

Thus given any $\boldsymbol{g}$ we can find an $\boldsymbol{s}$ such that (2) is equivalent to (1). The constraint $\boldsymbol{s}'\boldsymbol{1} = 1$ can be justified on different grounds. The matrix $\boldsymbol{D}$ is not p.s.d. because it has zero trace, so that for some vector $\boldsymbol{u}$

$$\boldsymbol{u}'\boldsymbol{F}\boldsymbol{u} = \{(\boldsymbol{I} - \boldsymbol{s}\boldsymbol{1}')\boldsymbol{u}\}'\boldsymbol{D}\{(\boldsymbol{I} - \boldsymbol{s}\boldsymbol{1}')\boldsymbol{u}\} < 0$$

unless $\det(\boldsymbol{I} - \boldsymbol{s}\boldsymbol{1}') = 0$. Thus $\boldsymbol{F}$ is never p.s.d. when $\det(\boldsymbol{I} - \boldsymbol{s}\boldsymbol{1}') \neq 0$ which implies that only the case when $\boldsymbol{s}'\boldsymbol{1} = 1$ is worth considering. When $\boldsymbol{D}$ is singular $\boldsymbol{s}$ must not be chosen in the null-space of $\boldsymbol{D}$, else $\boldsymbol{D}\boldsymbol{s} = 0$ and (2) equates $\boldsymbol{F}$ to $\boldsymbol{D}$ which is not p.s.d.

The above has shown that if there exists $\boldsymbol{s}$, such that $\boldsymbol{s}'\boldsymbol{1} = 1$ and $\boldsymbol{s}'\boldsymbol{D} \neq 0$ and $\boldsymbol{F}$ given by (2) is p.s.d., then D is Euclidean. However, it has not yet been demonstrated that this is a necessary condition. To do so consider the vector t such that $t'\mathbf{1} = 1$, then

$$(I - \mathbf{1}t')(I - \mathbf{1}s') = I - \mathbf{1}t' \tag{3}$$

and

$$(I - \mathbf{1}t')F(I - t\mathbf{1}') = (I - \mathbf{1}t')D(I - t\mathbf{1}').$$

This shows that if (2) is p.s.d. for some s such that $s'\mathbf{1} = 1$ and $s'D \neq 0$ then it is p.s.d. for all such s. Since for D to be Euclidean F must be p.s.d. for some s, we have now shown that it must be p.s.d. for all s. Thus we have shown the following.

Theorem 2. D is Euclidean iff (2) is p.s.d. for any s such that $s'\mathbf{1} = 1$ and $s'D \neq 0$.

From this theorem we can derive a result given by Blumenthal (1970). When F is p.s.d. then for all non-zero vectors x, $x'Fx \geq 0$. When $y'\mathbf{1} = 0$ we can set $x = y$ to give $y'Dy = y'Fy \geq 0$. Conversely if $y'Dy \geq 0$, for all y such that $y'\mathbf{1} = 0$ one may set $y = (I - s\mathbf{1}')x$ for arbitrary x and $x'\mathbf{1} = 1$. Hence $x'Fx \geq 0$ for all x. Thus a different way of expressing necessary and sufficient conditions for D to be Euclidean is that $y'Dy \geq 0$ for all y such that $y'\mathbf{1} = 0$. This form is less convenient for constructive work than the version based on (2) given above.

The geometrical interpretation of (3) is straightforward. From (2) it follows that $(I - \mathbf{1}t')YY'(I - t\mathbf{1}')$ gives a new set of coordinates in which the origin is translated from the origin of Y by an amount $t'Y$. The interesting thing is that the starting origin of Y is irrelevant. After translation, the new origin is always such that $t'Y = 0$, a fact that will be exploited in the next section. Different decompositions may be used to give different orientations of axes for the two solutions, but these have no effect on the amount of translation. Thus all the solutions generated by different values of s are equivalent (as they must be) and represent translations in the smallest space that holds the coordinates. These equivalent solutions correspond to only a subset of those generated by g, which allows Y to be represented in more dimensions than the minimum required. Further, even when D is Euclidean g generates some inadmissible solutions as can be seen by taking $g = 0$. From (1) we have that $2g = \mathrm{diag}(YY')\mathbf{1}$ showing that $2g_i$ gives the squared distance of P_i from the origin and hence must be positive, but there are further constraints on acceptable values of g. The exact relation between g and s is complex, but when $\det D \neq 0$ things simplify to give some interesting results. Equating the diagonal elements of (1) and (2) gives

$$g = \tfrac{1}{2}(s'Ds)\mathbf{1} - Ds$$

so that

$$s = \tfrac{1}{2}(s'Ds)D^{-1}\mathbf{1} - D^{-1}g$$

yielding a quadratic equation for $\alpha = \frac{1}{2}(s'Ds)$

$$\alpha^2\mathbf{1}'D^{-1}\mathbf{1} - 2\alpha(1 + \mathbf{1}'D^{-1}g) + g'D^{-1}g).$$

The condition for this equation to have equal roots is that

$$\Delta(g) \equiv (1 + \mathbf{1}'D^{-1}g)^2 - (\mathbf{1}'D^{-1}\mathbf{1})(g'D^{-1}g) = 0$$

which turns out to be equivalent to $s'\mathbf{1} = 1$ and allows s to be found for any g of suitable form:

$$s = \left[\frac{1 + \mathbf{1}'D^{-1}g}{\mathbf{1}'D^{-1}\mathbf{1}} \right] D^{-1}\mathbf{1} - D^{-1}g.$$

When the quadratic has unequal roots then $s'\mathbf{1} \neq 1$. With complex roots it turns out that the imaginary component of (2) vanishes and F has full rank, yielding solutions Y in more than the minimum number of dimensions. With real roots F has full rank and if p.s.d. exposes a seeming contradiction because, as shown above, (2) is only p.s.d. when $s'\mathbf{1} = 1$. Thus when D is Euclidean, such solutions are impossible and for all vectors g such that F is p.s.d. we have that:

$$(1 + \mathbf{1}'D^{-1}g)^2 \leq (\mathbf{1}'D^{-1}\mathbf{1})(g'D^{-1}g),$$

an inequality for Euclidean distances that challenges a direct proof. The quantity $\Delta(g)$ has a prominent role in the subsequent discussion.

To conclude this section consider the problem of multidimensional unfolding. Here data exist in the form of a $p \times q$ rectangular matrix B of distances that may be regarded as formed from the last p rows and first q columns of an otherwise unknown distance matrix D of order $p + q$. When D arises from distances between points in $r < n - 1$ dimensions it may be possible to find coordinates that generate B. Not much seems to be known of necessary or sufficient conditions for B to be Euclidean. When a solution exists then $r \leq \min(p, q)$. Schonemann (1970) requires that $\max(p, q) > \frac{1}{2}r(r + 3)$ for a unique solution to a set of equations that derive coordinates.

3. Some special cases

From (2) we have that $(s'Y)(s'Y)' = 0$ and hence that $s'Y = 0$. This implies that the origin is at a weighted mean of the coordinates Y, the weights being given by s. Two simple choices of s are (i) $s = \mathbf{1}/n$ which puts the origin at the centroid and (ii) $s = e_i$, the unit vector along the ith coordinate axis, which puts the origin at P_i. The first choice always satisfies $s'D \neq 0$, unless D is null, and the second choice only gives $s'D = 0$ when the ith row of D is 0, which is clearly a non-Euclidean case. With that proviso we have that D is Euclidean if and only if the two equivalent conditions

$$(I - 1/n\mathbf{1}\mathbf{1}')D(I - 1/n\mathbf{1}\mathbf{1}') \qquad \text{is p.s.d.} \tag{4}$$

and

$$(I - \mathbf{1}e_i')D(I - e_i\mathbf{1}') \qquad \text{is p.s.d.} \tag{5}$$

are true.

These results were obtained by Schoenberg (1935), a surprisingly late date for such a fundamental property of Euclidean geometry. When Y is obtained from (4) by spectral decomposition, we have the method known as classical scaling (Torgerson (1958)) or principal coordinate analysis (Gower (1966)) which is much used by statisticians, psychologists, ecologists, etc. When Y is approximated by Y_r by selecting only the r columns of Y that correspond to the r largest eigenvalues of F, the sum of squares of projections from the points P_i onto the selected subspace is minimized or, what is the same thing, Trace($Y_r' Y_r$) is maximized. It is this least-squares property that makes the method attractive to statisticians. Of course $\boldsymbol{Y}$ could be derived from (5) by spectral decomposition too, which has similar least-squares properties—but only for axes with origin P_i. The choice of centroid as origin given by (4) is globally optimal. Young and Householder (1938) used results based on (5).

Choices of origin other than the two just discussed have geometrical interest.

The circumcentre. If we can choose an origin C such that the distance $CP_i = R$ a constant, then this origin is equivalent to the circumcentre of a triangle. The vertices P_i lies on a hypersphere centre C, radius R. It is clear that diag($\boldsymbol{YY}'$) gives the squares of the distances of the vertices from the origin. Hence for the origin to be at the circumcentre we require that

$$\operatorname{diag}(\boldsymbol{I} - \mathbf{1}\boldsymbol{s}')\boldsymbol{D}(\boldsymbol{I} - \boldsymbol{s}\mathbf{1}') = R^2\boldsymbol{I}$$

i.e.

$$(\boldsymbol{s}'\boldsymbol{D}\boldsymbol{s})\mathbf{1} - 2\boldsymbol{D}\boldsymbol{s} = R^2\mathbf{1}$$

where the diagonal has been expressed as a column-vector. Clearly $\boldsymbol{s}$ must be proportional to $\boldsymbol{D}^{-1}\mathbf{1}$ and because we require $\boldsymbol{s}'\mathbf{1} = 1$ we have that

$$\boldsymbol{s} = \boldsymbol{D}^{-1}\mathbf{1}/\mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1}$$

which gives

$$R^2 = -(\mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1})^{-1}. \tag{6}$$

Notice that this rather remarkable formula requires $\det(\boldsymbol{D}) \neq 0$, that is that the points are not degenerate, lying in fewer than $(n-1)$ dimensions. Whether this choice of weights $\boldsymbol{s}$ is of statistical interest is doubtful because of its sensitivity to ill-conditioned matrices $\boldsymbol{D}$. Perhaps R^2 might be a useful measure of the condition of $\boldsymbol{D}$.

The incentre. The incentre is the point that is equidistant from the faces of the configuration $P_1, P_2, \ldots, P_n$. The faces are the hyperplanes opposite each of the n vertices, e.g. the face opposite P_1, contains $P_2, P_3, \ldots, P_n$, etc. The equal distance r, say, referred to above, is the radius of the inhypersphere. To find r and the setting of $\boldsymbol{s}$ that places the origin at the incentre requires the equations for the faces. Referring the vertices to their principal axes gives a particularly simple representation where the co-ordinates of P_i are given by the ith row of $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\Lambda}^{1/2}$ where $\boldsymbol{YY}' = \boldsymbol{X}'\boldsymbol{\Lambda}\boldsymbol{X} = (\boldsymbol{I} - \mathbf{1}\mathbf{1}'/n)\boldsymbol{D}(\boldsymbol{I} - \mathbf{1}\mathbf{1}'/n)$ and $\boldsymbol{Y}'\boldsymbol{Y} = \boldsymbol{\Lambda}$, the diagonal matrix of eigenvalues of $\boldsymbol{YY}'$. Thus we have chosen $\boldsymbol{s} = \mathbf{1}/n$ with the spectral decomposition. Note that the columns of $\boldsymbol{X}$ are eigenvectors of $\boldsymbol{YY}'$ and hence are orthogonal, apart from a final column $\mathbf{1}/\sqrt{n}$.

The equation of a plane has the form $l_1x_1 + l_2x_2 + \cdots + l_{n-1}x_{n-1} = p$. We recall that the normal to the plane has direction cosines proportional to $(l_1, l_2, \ldots, l_{n-1})$ and that the point with coordinates $(u_1, u_2, \ldots, u_{n-1})$ is distant $H(l_1u_1 + l_2u_2 + \cdots + l_{n-1}u_{n-1} - p)$ from the plane where the normaliser H is given by $H^{-2} = \sum_{i=1}^{n-1} l_i^2$. With these considerations in mind consider the plane

$$\lambda_1^{-1/2}x_{11}x_1 + \lambda_2^{-1/2}x_{21}x_2 + \cdots + \lambda_{n-1}^{-1/2}x_{n-1,1}x_{n-1} = -1/n.$$

Direct substitution of $P_i = (\lambda_1^{1/2}x_{i1}, \lambda_2^{1/2}x_{i2}, \ldots, \lambda_{n-1}^{1/2}x_{i,n-1})$ and using the orthogonality relationships, shows that this plane contains P_i for $i = 2, 3, \ldots, n$ and so it is the equation of the face opposite P_1. In passing, it is interesting to note the duality between the coordinates of P_1 and the direction cosines of the normal to the opposite face, which differ only in the scalings $\lambda_i^{1/2}$ and $\lambda_i^{-1/2}$. In fact to give direction cosines, the coefficients have to be normalized to have unit sum-of-squares. P_1 may be replaced by any vertex and the equations for the opposite face written down. The set of normalisers is then given by $\boldsymbol{H}^{-2} = \operatorname{diag}(\boldsymbol{X\Lambda}^{-1}\boldsymbol{X}')$ and the equation for the ith face has to be multiplied by H_i, the square root of the ith diagonal value of $\boldsymbol{H}^2$. To evaluate $\boldsymbol{H}$ observe that $(\boldsymbol{X}, \mathbf{1}/\sqrt{n})$ is orthogonal, so that

$$(\boldsymbol{X}\mathbf{1}/\sqrt{n})\begin{bmatrix}\boldsymbol{\Lambda} & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}\boldsymbol{X}'\\ \mathbf{1}'/\sqrt{n}\end{bmatrix} = \boldsymbol{X\Lambda X}' + \mathbf{11}'/n$$

has inverse:

$$(\boldsymbol{X}\mathbf{1}/\sqrt{n})\begin{bmatrix}\boldsymbol{\Lambda}^{-1} & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}\boldsymbol{X}'\\ \mathbf{1}'/\sqrt{n}\end{bmatrix} = \boldsymbol{X\Lambda}^{-1}\boldsymbol{X}' + \mathbf{11}'/n.$$

Thus

$$\begin{aligned}\boldsymbol{X\Lambda}^{-1}\boldsymbol{X}' &= (\boldsymbol{X\Lambda X}' + \mathbf{11}'/n)^{-1} - \mathbf{11}'/n\\ &= \{(\boldsymbol{I} - \mathbf{11}'/n)\boldsymbol{D}(\boldsymbol{I} - \mathbf{11}'/n) + \mathbf{11}'/n\}^{-1} - \mathbf{11}'/n\\ &= \boldsymbol{D}^{-1} - \frac{\boldsymbol{D}^{-1}\mathbf{11}'\boldsymbol{D}^{-1}}{\mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1}}\end{aligned}$$

the final step of which can be verified by direct multiplication.

Thus

$$\boldsymbol{H}^{-2} = \operatorname{diag}\left\{\boldsymbol{D}^{-1} - \frac{\boldsymbol{D}^{-1}\mathbf{11}'\boldsymbol{D}^{-1}}{\mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1}}\right\}. \tag{7}$$

The quantities H_i have a direct geometrical interpretation which follows from noting that the altitude from P_1 has length $h_1 = H_1$. Thus the normalizers are the corresponding altitudes.

If now $\boldsymbol{x}$ gives the co-ordinates of the incentre, relative to the principal axes, and r the radius of the insphere we have that

$$\boldsymbol{H}(\boldsymbol{X\Lambda}^{-1/2}\boldsymbol{x} + 1/n\mathbf{1}) = r\mathbf{1}$$

or

$$(\boldsymbol{HX\Lambda}^{-1/2}, -\mathbf{1})\begin{bmatrix}\boldsymbol{x}\\ r\end{bmatrix} = -1/n\boldsymbol{H}\mathbf{1}.$$

This linear equation has solution

$$\begin{bmatrix}\boldsymbol{x}\\ r\end{bmatrix} = \begin{bmatrix}\boldsymbol{\Lambda}^{1/2}\boldsymbol{X}'\boldsymbol{H}^{-1}\mathbf{1}\\ 1\end{bmatrix}\bigg/(\mathbf{1}'\boldsymbol{H}^{-1}\mathbf{1}) \tag{8}$$

as can be verified by direct substitution.

Thus the coordinates of the incentre are

$$x = Y'H^{-1}\mathbf{1}/\mathbf{1}'H^{-1}\mathbf{1} \tag{9}$$

and the inradius is

$$r = (\mathbf{1}'H^{-1}\mathbf{1})^{-1}. \tag{10}$$

This equation may also be written

$$r = (\sum 1/h_i)^{-1} \tag{11}$$

expressing the inradius in terms of the altitudes. The equation for x gives the translation from the centroid required to place the origin at the incentre. This requires setting $s = H^{-1}\mathbf{1}/\mathbf{1}'H^{-1}\mathbf{1}$ in (2), which satisfies $\mathbf{1}'s = 1$, as it should.

It is also possible to find the various excentres in which the hypersphere touches one face externally and the others internally. This requires

$$H(X\Lambda^{-1/2} + 1/n\mathbf{1}) = r_1(-2e_1 + \mathbf{1}) \qquad \text{or} \qquad (HX\Lambda^{-1/2}, 2e_1 - \mathbf{1})\begin{bmatrix} x_1 \\ r_1 \end{bmatrix} = -1/nH\mathbf{1}$$

which has solution

$$x_1 = Y'H^{-1}(\mathbf{1} - 2e_1)/\mathbf{1}'H^{-1}(\mathbf{1} - 2e_1) \tag{12}$$

and

$$r_1 = \{\mathbf{1}'H^{-1}(\mathbf{1} - 2e_1)\}^{-1}$$

and hence $r_1^{-1} = r^{-1} - 2h_1^{-1}$ and similar expressions for $r_2, r_3, \ldots, r_n$. Summing the last expression and using (11) we have that

$$\sum_{i=1}^{n} r_i^{-1} = (n-2)r^{-1} \tag{13}$$

relating all the inradii. To centre at the ith excentre, set $s = H^{-1}(\mathbf{1} - 2e_i)/\mathbf{1}'H^{-1}(\mathbf{1} - 2e_i)$.

To conclude this section the special settings of s that have been discussed are gathered together in Table 1.

Table 1. Choices of origin and associated properties

s	Origin at	Other properties
$\mathbf{1}/n$	Centroid	
e_i	P_i	
$D^{-1}\mathbf{1}/\mathbf{1}'D^{-1}\mathbf{1}$	Circumcentre	$R = -(\mathbf{1}'D^{-1}\mathbf{1})^{-1}$
$H^{-1}\mathbf{1}/\mathbf{1}'H^{-1}\mathbf{1}$	Incentre	$r = (\mathbf{1}'H^{-1}\mathbf{1})^{-1}$
$H^{-1}v_i/\mathbf{1}'H^{-1}v_i$	ith excentre	$r_i = (\mathbf{1}'H^{-1}v_i)^{-1}$

where $H^{-2} = \operatorname{diag}\left(D^{-1} - \dfrac{D^{-1}\mathbf{1}\mathbf{1}'D^{-1}}{\mathbf{1}'D^{-1}\mathbf{1}}\right)$ and $v_i = (\mathbf{1} - 2e_i)$.

Many of the quantities required in Table 1 can be produced from the single matrix inversion

$$C^{-1} \equiv \begin{bmatrix} D & \mathbf{1} \\ \mathbf{1}' & 0 \end{bmatrix}^{-1} = \begin{bmatrix} D^{-1} - \dfrac{D^{-1}\mathbf{1}\mathbf{1}'D^{-1}}{\mathbf{1}'D^{-1}\mathbf{1}} & \dfrac{D^{-1}\mathbf{1}}{\mathbf{1}'D^{-1}\mathbf{1}} \\ \dfrac{\mathbf{1}'D^{-1}}{\mathbf{1}'D^{-1}\mathbf{1}} & \dfrac{-1}{\mathbf{1}'D^{-1}\mathbf{1}} \end{bmatrix}.$$

4. Content

It has already been noted in Section 2 that the Euclideanarity of $\boldsymbol{D}$ can be decided by evaluating the contents of increasing sets of vertices $P_1, P_2, P_3, \ldots, P_r$ $(r = 2, 3, \ldots, n)$. The basic formula for the content C_n of n points, whose coordinates are the rows of $\boldsymbol{Y}$, is $(n-1)!C_n = \det(\boldsymbol{Y}, \mathbf{1})$ for which it is essential that $\boldsymbol{Y}$ has $(n-1)$ columns and has rank $(n-1)$, so that $\boldsymbol{D}$ is not degenerate. When $n = 2$, $C_2 = d_{12}$ the length of the line joining P_1 and P_2. Similarly C_3 is the area of the triangle with vertices P_1, P_2, P_3 and C_4 is the volume of the tetrahedron P_1, P_2, P_3, P_4, etc. It follows trivially from the definition that

$$(n-1)!^2 C_n^2 = \det \begin{bmatrix} \boldsymbol{Y}' \\ \mathbf{1}' \end{bmatrix} (\boldsymbol{Y} \quad \mathbf{1})$$
$$= \det \begin{bmatrix} \boldsymbol{Y}'\boldsymbol{Y} & \boldsymbol{Y}'\mathbf{1} \\ \mathbf{1}'\boldsymbol{Y} & n \end{bmatrix}.$$

The particular orientation and translation of $\boldsymbol{Y}$ do not affect content so without loss of generality we may assume that $\boldsymbol{Y}$ is referred to its principal axes through the centroid. Thus $\boldsymbol{Y}'\mathbf{1} = 0$ and $\boldsymbol{Y}'\boldsymbol{Y} = \boldsymbol{\Lambda}$ the diagonal matrix of eigenvalues. Thus we have the well-known result that

$$(n-1)!^2 C_n^2 = n\lambda_1\lambda_2 \ldots \lambda_{n-1}.$$

However, for our purposes it is more useful, and certainly much more informative, to evaluate C_n^2 by reversing the order of the product in C_n^2 to give

$$(n-1)!^2 C_n^2 = \det(\boldsymbol{Y}\boldsymbol{Y}' + \mathbf{1}\mathbf{1}') = \det(\boldsymbol{F} + \mathbf{1}\mathbf{1}')$$

where $\boldsymbol{Y}$ is now general once again.

Formally we may substitute (1) for $\boldsymbol{F}$ to give after some manipulation

$$(n-1)!^2 C_n^{+2} = \det \boldsymbol{D}[\Delta(g) + \mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1}]. \tag{14}$$

The quantity C_n^+ will be termed pseudocontent because it embraces invalid settings when $\boldsymbol{F}$ is of rank n. True content should not depend on the arbitrary vector $\boldsymbol{g}$, so this expression gives an alternative derivation of the condition $\Delta(g) = 0$ for the rank of $\boldsymbol{Y}$ to be $n - 1$.

An immediate consequence of (14) is that

$$(n-1)!^2 C_n^2 = \det \boldsymbol{D}(\mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1})$$
$$= -\det \boldsymbol{D}/R^2 \tag{15}$$

It is easy to see that det $\boldsymbol{D}(\mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1})$ may be evaluated as det $\boldsymbol{C}$ the determinant of $\begin{bmatrix} \boldsymbol{D} & \mathbf{1} \\ \mathbf{1}' & 0 \end{bmatrix}$ giving another expression for content and incidentally yet another use of this matrix, whose inverse we have already seen yields so many useful properties.

When $\Delta(g) \neq 0$, $\boldsymbol{Y}$ is of full rank n and the geometrical significance of pseudocontent needs to be identified. In the derivation of (14), $\boldsymbol{D}$ may now be replaced by $\boldsymbol{F}$ so that we are looking for geometrical interpretations for det $\boldsymbol{F}$, $\Delta(g)$ and $\mathbf{1}'\boldsymbol{F}^{-1}\mathbf{1}$. The points $P_1, P_2, \ldots, P_n$ still lie in an $(n-1)$-dimensional hyperplane and have content C_n. Suppose this hyperplane is distance d from the origin. The content of points $P_1, P_2, \ldots, P_n$ together with the origin 0 is $(1/n!)$ det $\boldsymbol{Y}$, where $\boldsymbol{Y}$ is $n \times n$ with rank n.

For example $\frac{1}{2}\begin{vmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{vmatrix}$ is the area of the triangle OP_1P_2. Now this area may be expressed as the product of half the content of the base with the altitude from O. In general $(1/n!)$ det $\boldsymbol{Y}$ is the product of $1/n$ times content of the 'base' (i.e. C_n/n) with the altitude from O (i.e. d).

Thus

$$\det \boldsymbol{Y} = (n-1)!C_n d$$

and

$$\det \boldsymbol{F} = (\det \boldsymbol{Y})^2 = ((n-1)!C_n d)^2.$$

This identifies det $\boldsymbol{F}$ but suggests that an expression for d might be useful. Such an expression is found in the next paragraph.

All points lying in the hyperplane of $\boldsymbol{Y}$ will have coordinates $\boldsymbol{l}'\boldsymbol{Y}$ where $\boldsymbol{l}$ ranges over all values such that $\boldsymbol{l}'\mathbf{1} = 1$. Hence d^2 is the minimum value of $\boldsymbol{l}'\boldsymbol{Y}\boldsymbol{Y}'\boldsymbol{l} = \boldsymbol{l}'\boldsymbol{F}\boldsymbol{l}$. Thus d is the minimum of the Lagrangian $\boldsymbol{l}'\boldsymbol{F}\boldsymbol{l} - 2\lambda(\boldsymbol{l}'1 - 1)$. Differentiating with respect to $\boldsymbol{l}$ gives $\boldsymbol{F}\boldsymbol{l} = \lambda\mathbf{1}$ and therefore $\lambda = \boldsymbol{l}'\boldsymbol{F}\boldsymbol{l} = d^2$ and $\boldsymbol{l} = \lambda\boldsymbol{F}^{-1}\mathbf{1}$. Hence

$$\mathbf{1}'\boldsymbol{l} = 1 = d^2(\mathbf{1}'\boldsymbol{F}^{-1}\mathbf{1})$$

and

$$d^2 = (\mathbf{1}'\boldsymbol{F}^{-1}\mathbf{1})^{-1}. \tag{16}$$

This identifies $\mathbf{1}'\boldsymbol{F}^{-1}\mathbf{1}$.

Using the formula $(n-1)!^2 C_n^{+2} = \det(\boldsymbol{F} + \mathbf{1}\mathbf{1}')$ when $\boldsymbol{F}$ is non-singular gives

$$\begin{aligned}(n-1)!^2 C_n^{+2} &= \det \boldsymbol{F}(1 + \mathbf{1}'\boldsymbol{F}^{-1}\mathbf{1}) \\ &= \det \boldsymbol{F}(1 + 1/d^2)\end{aligned}$$

i.e.

$$C_n^{+2} = C_n^2(1 + d^2) \tag{17}$$

relating the pseudocontent C_n^+ to the true content C_n.

Comparing (17) with (14) identifies $\Delta(g)$ to give

$$\begin{aligned}\Delta(g) &= d^2\mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1} = -d^2/R^2 \qquad (18) \\ &= \mathbf{1}'\boldsymbol{D}^{-1}\mathbf{1}/\mathbf{1}'\boldsymbol{F}^{-1}\mathbf{1}.\end{aligned}$$

The geometrical meaning of $\Delta(g)$ is now clear. When $\Delta(g)=0$ then $d=0$ and $\boldsymbol{Y}$ is represented in $(n-1)$ dimensions that contain the origin, which corresponds to (2), where $\boldsymbol{s}'\boldsymbol{Y}=0$ identifies the origin. When $\Delta(g)<0$ then $d^2>0$ and the origin is outside the space containing $P_1, P_2, \ldots, P_n$. When $\Delta(g)>0$, d^2 is negative and $\boldsymbol{Y}$ cannot yield a real Euclidean representation.

Let us now consider a matrix $\boldsymbol{F}$ of form (2) and consider the problem of evaluating the content C_{n-1} of a face, obtained by dropping, say, the last row and column of $\boldsymbol{D}$. Clearly $\boldsymbol{F}_{n-1}$ the leading $(n-1)$ principal minor of $\boldsymbol{F}$ contains all the information needed to reconstruct the leading $(n-1)$-minor of $\boldsymbol{D}$, and indeed also the deleted row and column. $\boldsymbol{F}_{n-1}$ is not admissible so we have that

$$(n-2)!^2 C_{n-1}^{+2} = \det \boldsymbol{F}_{n-1}(1+\mathbf{1}'\boldsymbol{F}_{n-1}^{-1}\mathbf{1}) = \det \boldsymbol{F}_{n-1}(1+1/d^2)$$

where d is now to be identified as the altitude h_n from P_n.

From (17)

$$\begin{aligned}(n-2)!^2 C_{n-1}^2 &= \det \boldsymbol{F}_{n-1}/d^2 \\ &= \det \boldsymbol{F}_{n-1}(\mathbf{1}'\boldsymbol{F}_{n-1}^{-1}\mathbf{1}).\end{aligned} \tag{19}$$

This formula shows that the content of successively smaller subsets of vertices may be found from matrices of type (2) as well as from $\boldsymbol{D}$ itself, by using much the same formula.

To close this section a direct proof is given of the relationship (7) for the altitudes. We have seen that $(n-1)!^2 C_n^2 = \det \boldsymbol{C}$ and that $C_n = (n-1)^{-1} C_{n-1} h_i$ where C_{n-1} is now the content of the face opposite P_i and h_i is the corresponding altitude. Now $(n-2)!^2 C_{n-1}^2$ is given by $\det \boldsymbol{C}_i$, the ith principal minor of $\boldsymbol{C}$. Hence $\det \boldsymbol{C} = h_i^2 \det \boldsymbol{C}_i$ so that h_i^{-2} is the ith diagonal value of $\boldsymbol{C}^{-1}$ as required by (7).

5. Eigenvalue results

A simple algebraic result is useful. Defining $\Delta_\lambda(\boldsymbol{g})$ to be $\Delta(\boldsymbol{g})$ with $\boldsymbol{D}$ replaced by $\boldsymbol{D}-\lambda \boldsymbol{I}$, it is simple to show that

$$\Delta_\lambda(\boldsymbol{g}+\alpha\mathbf{1}) = \Delta_\lambda(\boldsymbol{g}) + 2\alpha\mathbf{1}'(\boldsymbol{D}-\lambda\boldsymbol{I})^{-1}\mathbf{1}.$$

Also

$$\det \boldsymbol{F} = \det(\boldsymbol{D}+\mathbf{1}\boldsymbol{g}'+\boldsymbol{g}\mathbf{1}') = \det \boldsymbol{D}\,\Delta(\boldsymbol{g}).$$

It follows that the characteristic equation of (1) is

$$\det(\boldsymbol{D}-\lambda\boldsymbol{I})\,\Delta_\lambda(\boldsymbol{g}) = 0 \tag{20}$$

and the characteristic equation of (2) is obtained from (20) by replacing $\boldsymbol{g}$ by $\frac{1}{2}(\boldsymbol{s}'\boldsymbol{D}\boldsymbol{s})\mathbf{1}-\boldsymbol{D}\boldsymbol{s}$ to give, after some manipulation,

$$\begin{aligned}&\lambda \det(\boldsymbol{D}-\lambda\boldsymbol{I})[\lambda\{\mathbf{1}'(\boldsymbol{D}-\lambda\boldsymbol{I})^{-1}\boldsymbol{s}\}^2 \\ &\quad -\lambda\mathbf{1}'(\boldsymbol{D}-\lambda\boldsymbol{I})^{-1}\mathbf{1}\boldsymbol{s}'(\boldsymbol{D}-\lambda\boldsymbol{I})^{-1}\boldsymbol{s} - \boldsymbol{s}'\boldsymbol{s}\mathbf{1}'(\boldsymbol{D}-\lambda\boldsymbol{I})^{-1}\mathbf{1}] = 0\end{aligned} \tag{21}$$

Thus (21) always has a zero eigenvalue (corresponding to the vector $\boldsymbol{s}$) showing that (2) always gives coordinates $\boldsymbol{Y}$ in, at most, $n-1$ dimensions. If $\boldsymbol{D}$ itself has zero eigenvalues then (2) has one more zero eigenvalue than $\boldsymbol{D}$ whenever $\boldsymbol{s}$ is not in the null space of $\boldsymbol{D}$. This reduction in rank can only be achieved by choosing $\boldsymbol{g}$ to make (1) compatible with (2) and then it gives the greatest reduction possible. Geometrically, (2) generates coordinates $\boldsymbol{Y}$ of points in the minimal dimensioned space. From (20) and (21) it follows that the smallest eigenvalue of $\boldsymbol{F}$ is never greater than the second-smallest eigenvector of $\boldsymbol{D}$. Hence for $\boldsymbol{D}$ to be Euclidean it is necessary, though not sufficient, for $\boldsymbol{D}$ to have only one negative eigenvalue.

When (2) has p (say) positive and q (say) negative eigenvalues, a Euclidean representation is not possible. It may then be asked, what is the maximal subset of the points $P_1, P_2, \ldots, P_n$ that is Euclidean? A plausible conjecture is that this subset is of size $p+1$, but Fig. 2 gives a counterexample. For the 'tetrahedron' of Fig. 2, (21) has two positive eigenvalues, one negative eigenvalue and the mandatory zero eigenvalue. Thus $p+1=3$ and the conjecture requires at least one closed triangle in the configuration. No such triangle exists.

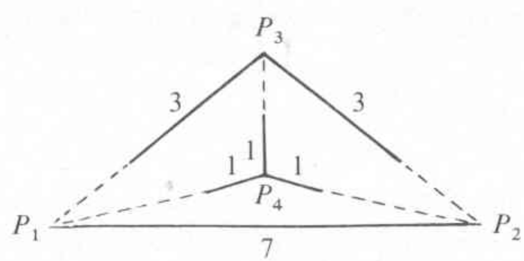

Fig. 2. In this configuration no triangle is closed but the number of positive eigenvalues of (21) is 2.

The structure of Fig. 2 may be generalised to n points, by having one side of length a_1, joined to two sides of length a_2, joined to three sides of length a_3, and so on. We can ensure that no triangle is closed by requiring that $a_i > 2a_{i+1}$ for $i = 1, 2, \ldots, n-2$. With this configuration it may be shown that the minimum number of positive eigenvalues of (21) is $\frac{1}{2}n$, obtained when the signs alternate $(+ - + - + - \cdots)$, and the maximum number is about $2n/3$, obtained with the following sequence of signs $(+ - +, + - +, + - +, \cdots)$. What happens with less regular structures is not known but the above results are sufficient to indicate that there is no simple relationships between the number of positive eigenvalues and the size of maximal Euclidean subsets of points.

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