Distance Geometry

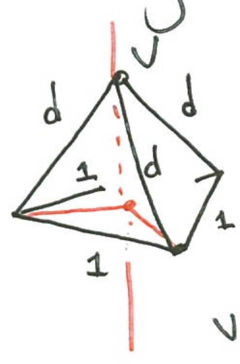
We now consider a fundamental question: given $\binom{n}{2}$ positive numbers d_{ij}, when are they the pairwise distances between n points in $\mathbb{R}^{n+1}$?

~~Two~~ A few observations are immediate:

1) $d_{ij} + d_{jk} - d_{ik} \geq 0$ for all i, j, k

2) If the points lie in a ~~smaller~~ lower dimensional subspace, we must have more relations.

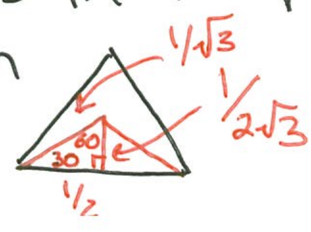
3) There are more relations than the triangle inequalities



We must have

$$d > \frac{1}{\sqrt{3}}$$

as in the planar version



and the vertex v must lie on the line through the center of the planar case.

However, for ~~d~~

$$\frac{1}{\sqrt{3}} > d > 1/2$$

the triangle inequalities are still satisfied, but no such tetrahedron exists.

Definition. A matrix in the form

$$\begin{pmatrix} 0 & -\frac{d_{12}^2}{2} & \cdots & \\ -\frac{d_{21}^2}{2} & 0 & & \\ \vdots & & \ddots & \\ \vdots & & & 0 \end{pmatrix} = D$$

will be called a distance matrix. The d_{ij} are distances between points i and j.

Cayley-Menger Determinant

A determinant that gives the volume of a simplex in j dimensions. If S is a j-simplex in $\mathbb{R}^n$ with vertices $v_1, \ldots, v_{j+1}$ and $B = (\beta_{ik})$ denotes the $(j+1)\times(j+1)$ matrix given by

$$\beta_{ik} = |v_i - v_k|_2^2, \qquad (1)$$

then the content V_j is given by

$$V_j^2(S) = \frac{(-1)^{j+1}}{2^j (j!)^2} \det(\hat{B}), \qquad (2)$$

where $\hat{B}$ is the $(j+2)\times(j+2)$ matrix obtained from B by bordering B with a top row $(0, 1, \ldots, 1)$ and a left column $(0, 1, \ldots, 1)^T$. Here, the vector L2-norms $|v_i - v_k|_2$ are the edge lengths and the determinant in (2) is the Cayley-Menger determinant (Sommerville 1958, Gritzmann and Klee 1994). The first few coefficients for $j = 0, 1, \ldots$ are -1, 2, -16, 288, -9216, 460800, ... (OEIS A055546).

For $j = 2$, (2) becomes

$$-16\,\Delta^2 = \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & c^2 & b^2 \\ 1 & c^2 & 0 & a^2 \\ 1 & b^2 & a^2 & 0 \end{vmatrix}, \qquad (3)$$

which gives the area for a plane triangle with side lengths a, b, and c, and is a form of Heron's formula.

For $j = 3$, the content of the 3-simplex (i.e., volume of the general tetrahedron) is given by the determinant

$$288\,V^2 = \begin{vmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2 \\ 1 & d_{21}^2 & 0 & d_{23}^2 & d_{24}^2 \\ 1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2 \\ 1 & d_{41}^2 & d_{42}^2 & d_{43}^2 & 0 \end{vmatrix}, \qquad (4)$$

where the edge between vertices i and j has length d_{ij}. Setting the left side equal to 0 (corresponding to a tetrahedron of volume 0) gives a relationship between the distances between vertices of a planar quadrilateral (Uspensky 1948, p. 256).

Buchholz (1992) gives a slightly different (and slightly less symmetrical) form of this equation.

SEE ALSO:
Heron's Formula, Quadrilateral, Tetrahedron

This entry contributed by Karen D. Colins

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We are now going to prove a useful characterization of the distance matrices that can actually be realized in Euclidean space.

Theorem (Gower, 1982)
D is Euclidean $\iff$ $(I-1s^T)D(I-s1^T)$ is positive semidefinite for all s with $s^T1=1$ and $s^TD \neq 0$.

Note: We will show that this $\Rightarrow$ $(I-1s^T)D(I-s1^T) = YY^T$ where Y are the coordinates of points!

~~Proof. ($\Leftarrow$)~~

~~Suppose D is Euclid~~

We start with something easier:

Claim. D is Euclidean $\iff$ $\exists$ a vector $\vec{g}$ so that $D + g1^T + 1g^T$ is positive semidefinite.

Proof. D is Euclidean $\iff$ $\exists$ vectors $\vec{Y}_1, \dots, \vec{Y}_n$ whose pairwise distances are the d_{ij}.

Assembling these $\vec{\gamma}_i$ into a matrix γ, the Gramian $\gamma\gamma^T$ is a matrix F of dot products

$$F = (\gamma\gamma^T)_{ij} = \langle \vec{\gamma}_i, \vec{\gamma}_j \rangle$$

so that

$$\begin{aligned} d_{ij}^2 &= \langle \vec{\gamma}_i - \vec{\gamma}_j, \vec{\gamma}_i - \vec{\gamma}_j \rangle \\ &= \langle \vec{\gamma}_i, \vec{\gamma}_i \rangle + \langle \vec{\gamma}_j, \vec{\gamma}_j \rangle - 2\langle \vec{\gamma}_i, \vec{\gamma}_j \rangle \\ &= f_{ii} + f_{jj} - 2f_{ij} \end{aligned}$$

Now ~~every matrix~~

F is symmetric and p.s.d. $\iff$ $F = \gamma\gamma^T$ or F is a gramian

positive semidefinite

So we have proved

D is Euclidean $\iff$ $\exists$ a symmetric p.s.d. F so that $d_{ij}^2 = f_{ii} + f_{jj} - 2f_{ij}$.

We now work more on the rhs.

Any symmetric F may be written

$$F = D + G$$

where G is symmetric. If, in addition

$$d_{ij}^2 = f_{ii} + f_{jj} - 2f_{ij}$$

then

$$d_{ij}^2 = \left(\cancel{0} - \cancel{\tfrac{1}{2} d_{ii}^2}^{\,0} + g_{ii}\right) + \left(-\cancel{\tfrac{1}{2} d_{jj}^2}^{\,0} + g_{jj}\right)$$
$$- 2\left(-\tfrac{1}{2} d_{ij}^2 + g_{ij}\right)$$
$$= d_{ij}^2 + g_{ii} + g_{jj} - 2g_{ij}$$

so we know

$$\tfrac{1}{2}(g_{ii} + g_{jj}) = \cancel{\tfrac{1}{2}(g_{ii} + 2g_{ij})} = g_{ij},$$

and if $\vec{g}$ is given by $\vec{g}_i = \frac{1}{2} g_{ii}$, then we have

$$F = D + g1^T + 1g^T.$$

Now (we claim) we're done. If D is Euclidean, $\exists$ such an $F = \Psi\Psi'$, and $F = D + G$ where G is as above. If $\exists$ a $\vec{g}$ so that $F = D + g1^T + 1g^T$ is p.s.d. (it is symmetric by construction), then F is a Gramian $F = \Psi\Psi^T$ and the pairwise distances between the Ψ are the d_{ij} by construction. $\square$

Claim. $\exists$ a vector $\vec{g}$ so that $D + g\mathbb{1}^T + \mathbb{1}g^T$ is positive semidefinite $\iff$ $\exists\ \vec{s}$ so that $s^T\mathbb{1} = 1$, $s^T D \neq 0$, and $(I - \mathbb{1}s^T)D(I - s\mathbb{1}^T)$ is positive semidefinite.

Proof. We know $D + g\mathbb{1}^T + \mathbb{1}g^T$ is symmetric by construction, so it is p.s.d. $\iff$ $D + g\mathbb{1}^T + \mathbb{1}g^T = \Psi\Psi^T$ for some Ψ. Further, $(I - \mathbb{1}s^T)D(I - s\mathbb{1}^T)$ is symmetric, so a similar statement holds.
So we show

$$\exists\ \vec{g} \text{ s.t. } D + g\mathbb{1}^T + \mathbb{1}g^T = \Psi\Psi^T \iff$$

$$\exists\ \vec{s} \text{ s.t. } (I - \mathbb{1}s^T)D(I - s\mathbb{1}^T) = \Psi_*\Psi_*^T$$

($\Rightarrow$) Given g, choose any s with $s^T\mathbb{1} = 1$, and $s^T g = 0$, and $s^T D \neq 0$.

n.b. What if D is rank 1 and g is the column space? ~~This can't happen b/c $g\mathbb{1}^T + g\mathbb{1}^T$ would~~

Then set $m = -Y^T s$ and let

$$Y_* = Y + 1m^T = Y - 1s^TY = (I - 1s^T)Y.$$

Then

$$Y_* Y_*^T = (I - 1s^T) Y Y^T (I - s1^T)$$

$$= (I - 1s^T)(D + g1^T + 1g^T)(I - s1^T)$$

$$= (I - 1s^T) D (I - s1^T)$$

$$+ (I - 1s^T)(g1^T + 1g^T)(I - s1^T)$$

But

$$(I - 1s^T)(g1^T + 1g^T)(I - s1^T) =$$

$$\underset{111}{g1^T} + \underset{112}{g\overset{1}{\cancel{1^T(-s}}1^T)} + \underset{121}{1g^T} + \underset{122}{1\overset{0}{\cancel{g^T(-s}}1^T)}$$

$$+ \underset{211}{(-1\overset{0}{\cancel{s^T)g}}1^T} + \underset{212}{(-1\overset{0}{\cancel{s^T)g}}1^T(-s1^T)} + \underset{221}{(-1\overset{1}{\cancel{s^T)(1}}g^T)}$$

$$+ \underset{222}{(-1s^T)(1\overset{0}{\cancel{g^T)(-s}}1^T)} = \cancel{g1^T} + \cancel{1g^T} - \cancel{g1^T} + \cancel{1g^T} - \cancel{1g^T}$$

$$= 0.$$

($\Leftarrow$) Going back is ~~harder~~ easier. If we are given s so that $s^T 1 = 1$, $s^T D \neq 0$, and $(I - 1s^T) D (I - s1^T) = \Psi_* \Psi_*^T$, we set

$$g = -Ds + \tfrac{1}{2} 1\, s^T \overset{D}{\,} s$$

$$g^T = -s^T D + \tfrac{1}{2} s^T \overset{D}{\,} s\, 1^T$$

Then

$$\begin{aligned}
\Psi_* \Psi_*^T &= (I - 1s^T) D (I - s1^T) \\
&= (D - 1s^T D)(I - s1^T) \\
&= D - Ds1^T - 1s^T D + 1 s^T s 1^T \\
&= D + \left(\tfrac{1}{2} 1 s^T s - Ds\right) 1^T \\
&\quad + 1\left(\tfrac{1}{2} s^T s 1^T - s^T D\right) \\
&= D + g1^T + 1g^T, \text{ as desired.}
\end{aligned}$$

$\square$

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

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