# Distance Geometry II.

We now have a constructive procedure for going from distances to points:

1) Choose $s$ so that $s^T D \neq 0$.

2) Rescale $s$ so that $s^T \mathbb{1} = 1$.

3) Take the SVD of $(I - s\mathbb{1}^T) D (I - \mathbb{1}s^T)$ to get $Q \Sigma Q^T$. Iff all the eigenvalues in the diagonal matrix $\Sigma$ are $\geq 0$, we can write this as

$$(Q\sqrt{\Sigma})(Q\sqrt{\Sigma})^T = YY^T$$

where $Y$ is a set of coordinates for points realizing the $d_{ij}$.

Proposition. If $\Psi\Psi^T = (I - 1s^T)\, D\, (I - s1^T)$, $s^T 1 = 1$, ~~then~~ and $s^T D \neq 0$, then $s^T \Psi = 0$.

Proof. We conjugate $\Psi\Psi^T$ by $s^T$ and $s$, so we have

$$
\begin{aligned}
(s^T\Psi)(\Psi^T s) &= s^T (I - 1s^T)\, D\, (I - s1^T)\, s \\
&= (s^T - \overset{1}{\cancel{s^T 1}}\, s^T)\, D\, (I - s1^T)\, s \\
&= 0
\end{aligned}
$$

or

$$(s^T\Psi)(s^T\Psi)^T = 0.$$

Thus $s^T\Psi = 0$. $\square$

Now

$$
\begin{aligned}
s^T\Psi &= [s_1 \cdots s_n] \begin{bmatrix} \longleftarrow \Psi_1 \longrightarrow \\ \vdots \\ \longleftarrow \Psi_n \longrightarrow \end{bmatrix} \\
&= s_1 \vec{\Psi}_1 + s_2 \vec{\Psi}_2 + \cdots + s_n \vec{\Psi}_n .
\end{aligned}
$$

So this means that the origin is at a weighted sum of the coordinates.

Example. Suppose $s = \frac{1}{n}\vec{1}$. In this case

$$s^T D = \left[\tfrac{1}{n} \cdots \tfrac{1}{n}\right]\left(-\tfrac{1}{2} d_{ij}^2\right)$$

$$= \left[-\tfrac{1}{2n}\sum_i d_{i1}^2 \quad -\tfrac{1}{2n}\sum_i d_{i2}^2 \quad \cdots \quad -\tfrac{1}{2n}\sum_i d_{in}^2\right]$$

which is clearly not $\vec{0}$ unless all the $d_{ij}^2 = 0$, so we can always make this choice.

Theorem. Given a point cloud with distances matrix $D$, the centered point cloud obtained by decomposing the p.s.d. matrix

$$\begin{bmatrix} 1-1/n & -1/n & \cdots & -1/n \\ -1/n & & & \\ -1/n & & & 1-1/n \end{bmatrix} D \begin{bmatrix} 1-1/n & -1/n & \cdots & \\ -1/n & & & \vdots \\ \vdots & & & 1-1/n \end{bmatrix}$$

into $YY^T$ is the principal component transform of the original cloud.

Further, if the eigenvalues of ~~those in~~ $\Sigma$, in the spectral decomposition of

$$(I - \tfrac{1}{n} 1 1^T)\, D\, (I - \tfrac{1}{n} 1 1^T) = Q \Sigma Q^T$$

are sorted in decreasing order, then the portion of $Q\sqrt{\Sigma}$ given by the first $r$ columns is the $r$-dimensional point cloud minimizing total sum of squares of projection distances.

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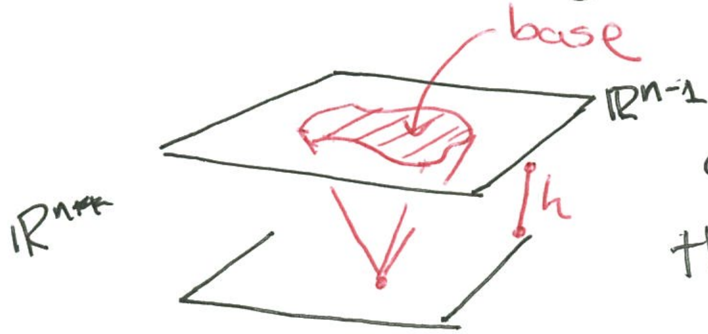
We now move to the ~~distance~~ volume formula. Now generally we have

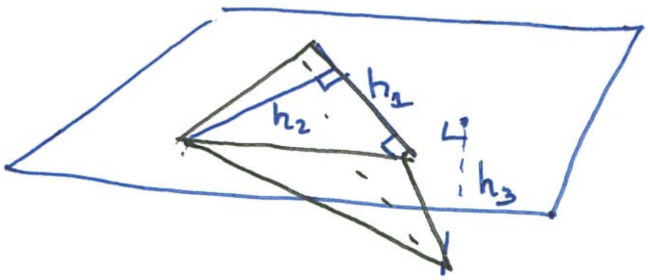



for the cone on any set $M$ in $\mathbb{R}^{n-1}$ that

$$\text{vol(cone)} = \frac{1}{n}\, \text{vol(base)} \cdot \text{height}$$

(The $1/n$ comes from the fact that we are integrating a scale factor $\lambda^{n-1}$ over the cone.)

This means we can compute recursively for a simplex




$$\mathrm{Vol} = \frac{1}{3}h_3 \cdot \frac{1}{2}h_2 \cdot \frac{1}{1}h_1$$

$$= \frac{1}{n!} h_n h_{n-1} \cdots h_1$$

where the $h_i$ are "heights" above subspaces containing lower dimensional faces.

To determine the heights start ~~with~~ by rigidly moving the entire arrangement of $(n+1)$ vertices so that $v_0$ is at the origin, and consider the square matrix $\begin{bmatrix} \leftarrow \vec{\varphi}_1 \rightarrow \vec{0} \\ \vdots \\ \leftarrow \vec{\varphi}_n \rightarrow \vec{0} \end{bmatrix} = \varphi_0$ (for "0 is ~~missing~~ at the origin").

We Know

$$\mathrm{Vol} = \frac{1}{n!} \det \begin{bmatrix} \varphi_0 \end{bmatrix} = \frac{1}{n!} \det \begin{bmatrix} \vec{\varphi}_1 - \vec{\varphi}_0 \\ \vec{\varphi}_2 - \vec{\varphi}_0 \\ \vec{\varphi}_n - \vec{\varphi}_0 \end{bmatrix}$$

Now by cofactor expansion along the bottom row

$$\det\begin{bmatrix} \vec{\psi}_1-\vec{\psi}_0 \\ \\ \vec{\psi}_n-\vec{\psi}_0 \end{bmatrix} = (-1)^{n-1}\det\left[\begin{array}{c|ccc} 1 & & \vec{\psi}_1-\vec{\psi}_0 & \\ 1 & & \vdots & \\ \vdots & & \vec{\psi}_n-\vec{\psi}_0 & \\ \hline 1 & 0 & \cdots & 0 \end{array}\right]$$

$$= (-1)^{n}\det\begin{bmatrix} 1 & \leftarrow \psi_0 \rightarrow \\ \vdots & \vdots \\ 1 & \leftarrow \psi_n \rightarrow \end{bmatrix}$$

adding $[0 \leftarrow \vec{\psi}_0 \rightarrow]$ to each row and swapping top and bottom rows.

Now we know $\det A = \det A^T$, so we can "square both sides" by writing

$$(\mathrm{Vol})^2 = \left(\frac{1}{n!}\right)^2 \det\begin{bmatrix} 1 & \leftarrow \vec{\psi}_0 \rightarrow \\ \\ 1 & \leftarrow \vec{\psi}_n \rightarrow \end{bmatrix}\begin{bmatrix} 1 & \cdots & 1 \\ \uparrow & & \uparrow \\ \psi_0 & & \psi_n \\ \downarrow & & \downarrow \end{bmatrix}$$

$$= \left(\frac{1}{n!}\right)^2 \det\begin{bmatrix} 1+\vec{\psi}_0\cdot\vec{\psi}_0 & & \\ & & \\ & & 1+\vec{\psi}_n\cdot\vec{\psi}_n \end{bmatrix}$$

again, we can augment this matrix by writing w/o changing the determinant

$$= \left(\frac{1}{n!}\right)^2 \det\begin{bmatrix} 1 & 1 & \longrightarrow & 1 \\ 0 & & & \\ \updownarrow & & 1+\vec{\psi}_i\cdot\vec{\psi}_j & \\ 0 & & & \end{bmatrix}$$

subtracting the top row from the others,

$$= \left(\frac{1}{n!}\right)^2 \det \begin{bmatrix} 1 & 1 & \cdots & 1 \\ -1 & & & \\ -1 & & \vec{\varphi}_i \cdot \vec{\varphi}_j & \\ & & & \\ -1 & & & \end{bmatrix}$$

Now the $(n+1)$ vectors $\varphi_0, \ldots, \varphi_n$ in $\mathbb{R}^n$ are clearly linearly dependent. So the determinant of their Gramian $[\vec{\varphi}_i \cdot \vec{\varphi}_j]$ is zero. That means the cofactor of the upper left "1" is zero and we can change that element w/o changing the determinant!

$$= \left(\frac{1}{n!}\right)^2 \det \begin{bmatrix} 0 & 1 & \cdots & 1 \\ -1 & & & \\ \vdots & & \vec{\varphi}_i \cdot \vec{\varphi}_j & \\ -1 & & & \end{bmatrix}$$

$$= -\left(\frac{1}{n!}\right)^2 \det \begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & & & \\ \vdots & & \vec{\varphi}_i \cdot \vec{\varphi}_j & \\ 1 & & & \end{bmatrix}$$

Now multiply the n+1 last columns by -2 and the top row by -½ to compensate,

$$= -\left(\frac{1}{n!}\right)^2 \left(\frac{1}{-2}\right)^{n+1} \cdot (-2) \det \begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & & & \\ \vdots & & -2\vec{Y}_i \cdot \vec{Y}_j & \\ 1 & & & \end{bmatrix}$$

$$= \frac{(-1)^{n+3}}{2^n} \left(\frac{1}{n!}\right)^2 \det \begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & & & \\ \vdots & & -2\vec{Y}_i \cdot \vec{Y}_j & \\ 1 & & & \end{bmatrix}$$

Now we can add any multiple of a row to any other row w/o changing det. So let's be clever and add

$$(Y_i \cdot Y_i) \cdot [0 \; 1 \cdots 1] \text{ to the } (i+1)\text{st row}$$

to get

$$= \frac{(-1)^{n+3}}{2^n} \left(\frac{1}{n!}\right)^2 \det \begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & & & \\ \vdots & & Y_i \cdot Y_i - 2Y_i \cdot Y_j & \\ 1 & & & \end{bmatrix}$$

and play ~~a~~ the ~~same~~ corresponding game with the columns to get

$$= \frac{(-1)^{n+3}}{2^n}\left(\frac{1}{n!}\right)^2 \det\begin{bmatrix} 0 & 1 & \cdots & 1 \\ \cancel{0} & & & \\ \vdots & & \vec{\psi}_i\cdot\vec{\psi}_i + \vec{\psi}_j\cdot\vec{\psi}_j - 2\vec{\psi}_i\cdot\vec{\psi}_j & \\ 1 & & & \end{bmatrix}$$

which is of course

$$= \frac{(-1)^{n+3}}{2^n}\left(\frac{1}{n!}\right)^2 \det\begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & & & \\ \vdots & & d_{ij}^2 & \\ 1 & & & \end{bmatrix}$$

Now there are $(n+1)$ columns that need to be multiplied by $-\frac{1}{2}$,

$$= \frac{(-1)^{n+3}}{2^n}\left(\frac{1}{n!}\right)^2 \det\begin{bmatrix} 0 & -1/2 & \cdots & -1/2 \\ 1 & & & \\ \vdots & & -\frac{1}{2}d_{ij}^2 = D & \\ 1 & & & \end{bmatrix} \cdot (-2)^{n+1}$$

$$= \frac{(-1)^3}{\cancel{(-2)^n}}\left(\frac{1}{n!}\right)^2 \det\begin{bmatrix} 0 & -1/2 & \cdots & -1/2 \\ 1 & & & \\ & & D & \\ 1 & & & \end{bmatrix} (-2)^{\cancel{n+}1}$$

$$= \frac{-1}{(n!)^2} \det \begin{bmatrix} 0 & \leftarrow 1 \rightarrow \\ 1 & \\ \updownarrow & D \\ 1 & \end{bmatrix}.$$

We have now proved the

Cayley-Menger Determinant Theorem.

~~Then~~ If $D$ is Euclidean, then the volume of the simplex given by the convex hull of the points is

$$(\mathrm{Vol})^2 = \frac{-1}{(n!)^2} \det \begin{bmatrix} 0 & 1 & 1 \\ 1 & & \\ & D & \\ 1 & & \end{bmatrix}$$

Thus, if $D$ is Euclidean,

$$\det \begin{bmatrix} 0 & 1 \cdots 1 \\ 1 & \\ \vdots & D \\ 1 & \end{bmatrix} \text{ is negative.}$$