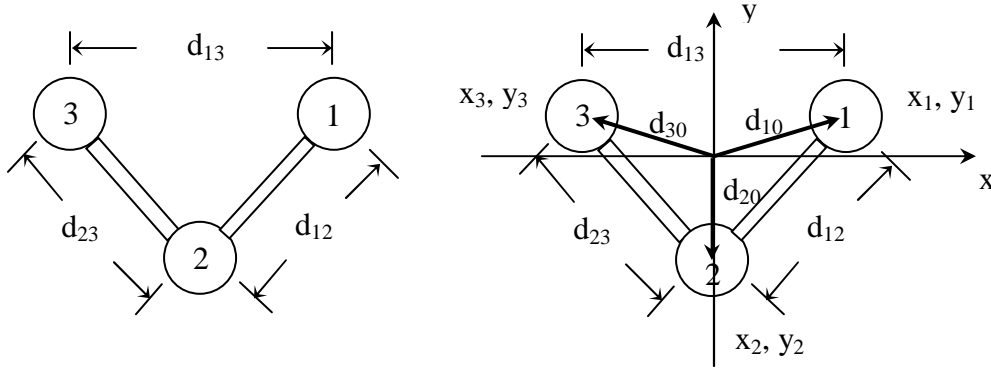


Metric Matrix Distance Geometry



Metric matrix with elements: $g_{ij} = x_i x_j + y_i y_j + z_i z_j$

centroid: $\sum x_i = 0$ $\sum y_i = 0$ $\sum z_i = 0$.

$$g_{ij} = \frac{1}{2} (d_{i0}^2 + d_{j0}^2 - d_{ij}^2)$$

$$d_{i0}^2 = \frac{1}{N} \sum_{j \neq i}^N d_{ij}^2 - \frac{1}{N^2} \sum_{j=1}^N \sum_{k>j}^N d_{jk}^2$$

$$d_{10}^2 = \frac{1}{3} (d_{12}^2 + d_{13}^2) - \frac{1}{3^2} (d_{12}^2 + d_{13}^2 + d_{23}^2)$$

example: $d_{12} = d_{23} = 5$ $d_{13} = 6$

$$d_{10}^2 = \frac{1}{3} (5^2 + 6^2) - \frac{1}{3^2} (5^2 + 6^2 + 5^2) = 10.777 \text{ or } d_{10} = 3.283$$

$$d_{20}^2 = \frac{1}{3} (5^2 + 5^2) - \frac{1}{3^2} (5^2 + 6^2 + 5^2) = 7.111 \text{ or } d_{20} = 2.667$$

$$g_{11} = \frac{1}{2} (d_{10}^2 + d_{10}^2) = 10.778$$

$$g_{12} = \frac{1}{2} (d_{10}^2 + d_{20}^2 - d_{12}^2) = -3.556$$

$$\mathbf{G} = \begin{pmatrix} 10.778 & -3.556 & -7.222 \\ -3.556 & 7.111 & -3.556 \\ -7.222 & -3.556 & 10.778 \end{pmatrix}$$

$\mathbf{G} \mathbf{w}_q = \lambda_q \mathbf{w}_q$ $q = x, y, \text{ or } z$

$$x_i = \lambda_1^{1/2} \mathbf{w}_{i1} \quad y_i = \lambda_2^{1/2} \mathbf{w}_{i2} \quad z_i = \lambda_3^{1/2} \mathbf{w}_{i3}$$

$$\lambda_1 = 18 \quad \mathbf{w}_1 = \begin{pmatrix} 0.707 \\ 0 \\ -0.707 \end{pmatrix}$$

$$\lambda_2 = 10.67 \quad \mathbf{w}_2 = \begin{pmatrix} 0.408 \\ -0.816 \\ 0.408 \end{pmatrix}$$

$$x_1 = 18^{1/2} 0.707 = 3$$

$$y_1 = 10.67^{1/2} 0.408 = 1.333$$

$$x_2 = 18^{1/2} 0 = 0$$

$$y_2 = 10.67^{1/2} -0.816 = -2.667$$

$$x_3 = 18^{1/2} -0.707 = -3$$

$$y_3 = 10.67^{1/2} 0.408 = 1.333$$