Classic (Metric) Multidimensional Scaling

- **This method was first systematized by Torgerson (building on earlier work by Householder, Eckart, Young in the 1930s), and subsequently improved by Gower (1966).**
- **It is basically a variation of principal components analysis and is also referred to as principal co-ordinates analysis. It is a three-step process:**
    - ♦ **Conversion of data (“distances”) into matrix of scalar products (B),**
    - ♦ **factoring/decomposing the resultant matrix of scalar-products to yield co-ordinates of points (up to similarity transform)**
    - ♦ **in a minimum number of dimensions, guaranteed to be an OLS fit to the data**

---

1. The proximity data are normalised and these normalised elements are squared:

$$d_{ij}^2 = d_{ij}^2 / \{\sum_i \sum_j d_{ij}^2 / p(p-1)\}$$

2. A scalar products matrix **B** is formed from the squared distances:

$$b_{ij} = [d_{ij}^2 - d_{i.}^2 - d_{.j}^2 + d_{..}^2]$$

where

$$d_{i.}^2 = \sum_j d_{ij}^2 / p$$

$$d_{.j}^2 = \sum_i d_{ij}^2 / p$$

$$d_{..}^2 = \sum_j d_{ij}^2 / p^2$$

3. **B** matrix is decomposed/factored using PCA to yield:

$$B = A \Lambda A'$$

- The eigenvectors **A** constitute the derived co-ordinates ... up to a **similarity** transform
    - *origin* of space is set to mean or centroid
    - any *orthogonal rotation/reflection* is permissible, so
    - it is *relative distance* which is retrieved).
  - **A** is positive semi-Gramian (with +ve latent roots λ_i) and hence representable in a real space
  - Rank(**A**) is the dimensionality necessary to reproduce the distances (usually p)

4. Eckart-Young (1936) show that if you want a solution in as small a dimension as possible ($q \ll p$), the *approximate solution :*

$$A_q \Lambda_q A'_q$$

Provides the basis for a OLS solution in q dimensions, with

$$X = A_q \Lambda_q^{1/2}$$

giving the co-ordinates.