Torgerson's Classical MDS derivation:
1: Determining Coordinates from Euclidean Distances

It is possible to construct a matrix **X** of Cartesian coordinates of points in Euclidean space when we know the Euclidean distances **D** amongst those points. To do this we take the following two steps:

1. Use the cosine law to convert **D** to a matrix **B** of "scalar products".
2. Perform a singular value decomposition of **B** to obtain **X**.

Cosine Law: For a triangle between points **i, j** and **k** in Euclidean space with sides $\mathbf{d_{ij}}$, $\mathbf{d_{ik}}$, and $\mathbf{d_{jk}}$, and angle $\theta_{\mathbf{jik}}$ between sides $\mathbf{d_{ij}}$ and $\mathbf{d_{ik}}$:

$$\mathbf{Cos}\ \theta_{\mathbf{jik}} = (\mathbf{d_{ij}}^2 + \mathbf{d_{ik}}^2 - \mathbf{d_{jk}}^2)/2\mathbf{d_{ij}}\mathbf{d_{ik}}$$

If we define $\mathbf{b_{jik}} = (\mathbf{d_{ij}}^2 + \mathbf{d_{ik}}^2 - \mathbf{d_{jk}}^2)/2$ then

$$\mathbf{b_{jik}} = \mathbf{d_{ij}}\mathbf{d_{ik}}\ \mathbf{Cos}\ \theta_{\mathbf{jik}}$$

The element $\mathbf{b_{jik}}$ is the *scalar product* (for points **j** and **k** relative to point **i**) of the vectors from point **i** to **j**, the vector from point **i** to **k**, and of **Cos** $\theta_{\mathbf{jik}}$**,** the cosine of the angle between the two vectors.

Singular Value Decomposition: The "scalar products" matrix $\mathbf{B_i}$ formed from the elements $\mathbf{b_{jik}}$ is a symmetric matrix which may be decomposed into singular values **V** (on diagonal) and singular vectors (column-wise) **U** such that

$$\mathbf{B_i} = \mathbf{UVU'}.$$

Furthermore, $\mathbf{B_i}$ is positive semidefinite, so, the rank of $\mathbf{B_i}$ (the number of positive eigen values) equals the dimensionality of **D,** and we may calculate

$$\mathbf{X}=\mathbf{UV}^{1/2}.$$

Then

$$\mathbf{B_i} = \mathbf{XX'}.$$

2: Determining Coordinates from Dissimilarities

If we have a matrix **D** of Euclidean distances amongst **n** points, we can use the two steps on the previous page to calculate the matrix **X** of the Cartesian coordinates of those points.

If we have a matrix **O** of observed dissimilarities which "approximate" Euclidean distances we can use two similar steps to calculate **X**.

1. **Calculate B:** The first step is to convert **O** into **B,** a matrix of "pseudo" scalar products, by "double centering" $\mathbf{O}^2$. Note:
   - The superscript on $\mathbf{O}^2$ means we double center the matrix of *squared* dissimilarities.
   - "Double centering" is subtracting the row and column means of the matrix from its elements, adding the grand mean and multiplying by -1/2. If **O** are error-free Euclidean distances, then **B** calculated this way are error-free scalar products relative to the origin.
2. **Singular Value Decomposition:** We double center **O** to obtain **B** because (see the next page for Torgerson's derivation) we can then determine the coordinates **X** by the singular value decomposition

   $$\mathbf{B = UVU'}$$

   which then permits us to calculate

   $$\mathbf{X=UV^{1/2}}.$$

Least Squares Properties of X: B is an indefinite matrix (it may have negative as well as zero or positive roots). It can be shown that if we define $\mathbf{V_r}$ by selecting the **r** largest singular values, and the corresponding singular vectors $\mathbf{U_r}$ and define:

$$\mathbf{X_r = U_r V_r^{1/2}}$$

then

$$\mathbf{B_r = X_r X_r'}$$

is a least squares approximation to **B.**

Torgerson's Double Centering Derivation

We begin with $\mathbf{B_i = XX'}$, the scalar products given earlier, where $\mathbf{B_i}$ is referred to an origin at point **i**. We translate the axes to the centroid of all points. This gives $\mathbf{X^*}$, a new set of Cartesian coordinates in the new system whose origin is at the centroid of the points. This translation is done by defining

$$\mathbf{c = (1'X)/n}$$

a **1xr** row vector of column means of **X**, where **1** is an **nx1** column vector of **n** one's.

We now define the centered $\mathbf{X^*}$ by subtracting the column means from elements of **X** by the equation

$$\mathbf{X^* = X - 1c = X - (11'X)/n} .$$

We can now define the scalar products of the centered configuration as

$$\begin{aligned}\mathbf{B^*} &= \mathbf{X^*X^{*\prime}} \\ &= \mathbf{(X - 1c)(X - 1c)' = (X - 1c)(X' - c'1')} \\ &= \mathbf{(X - 11'X/n)(X' - X'11'/n)} \\ &= \mathbf{(XX' - XX'11'/n - 11'XX'/n + 11'XX'11'/n^2)} \\ &= \mathbf{(B_i - B_i11'/n - 11'B_i/n + 11'B_i11'/n^2)} \\ &= \mathbf{(B_i - B_{i\,.} - B_{i\,.}' + B_{i\,..})}\end{aligned}$$

where $\mathbf{B_{i\,.}}$ is a matrix of (row or column) means of $\mathbf{B_i}$ and where $\mathbf{B_{i\,..}}$ contains the grand mean of all elements of $\mathbf{B_i}$.

Torgerson's Double Centering Derivation (continued)

The scalar version of the previous matrix equation allows us to see that an individual element of $\mathbf{B}^*$ is defined as:

$$b_{ij}^* = b_{ij} - \frac{1}{n}\sum_{k}^{n} b_{ik} - \frac{1}{n}\sum_{k}^{n} b_{kj} + \frac{1}{n^2}\sum_{g}^{n}\sum_{h}^{n} b_{gh} .$$

Noting that $b_{jk} = (d_{ij}^2 + d_{ik}^2 - d_{jk}^2)/2$, substituting and simplifying gives:

$$b_{ij}^* = -\frac{1}{2}\left[d_{ij}^2 - \frac{1}{n}\sum_{k}^{n} d_{ik}^2 - \frac{1}{n}\sum_{k}^{n} d_{kj}^2 + \frac{1}{n^2}\sum_{g}^{n}\sum_{h}^{n} d_{gh}^2 \right] .$$

That is, the scalar products of the centered coordinates are -1/2 times the squared distances with the row and column means removed and the grand mean added back in. As before, the singular value decomposition

$$\mathbf{B}^* = \mathbf{U}^*\mathbf{V}^*\mathbf{U}^{*\prime}$$

allows us to define:

$$\mathbf{X}^* = \mathbf{U}^*\mathbf{V}^{*1/2}.$$

3: Torgerson's Scalar Product Algorithm for Classical (Metric Unweighted) MDS

1. Let o_{ij} be the observed dissimilarity between stimuli i and j.
   d_{ij} be the Euclidean distance between stimuli i and j.
   x_i be the vector of coordinates of stimulus i on all dimensions.
   $x_. = 0$ denote the origin.
   $d_{i.}$ denote the distance from the origin to point i.
2. Assume that the data are error-free Euclidean distances: $o_{ij} = d_{ij}$.
3. Note: $o_{ij}^2 = d_{ij}^2 = (x_i - x_j)(x_i - x_j)' = x_i x_i' - 2x_i x_j' + x_j x_j'$,
   and: $o_{i.}^2 = d_{i.}^2 = x_i x_i' - 2x_i x_.' + x_. x_.' = x_i x_i'$.
4. If we define

   $$b_{ij} = -\frac{1}{2}(o_{ij}^2 - o_{i.}^2 - o_{.j}^2 + o_{..}^2) \quad ,$$

   then

   $$b_{ij} = -\frac{1}{2}[(x_i x_i' - 2x_i x_j' + x_j x_j') - x_i x_i' - x_j x_j'] = x_i x_j'.$$

   Thus we can solve for coordinates using the equality

   $$B = XX'.$$

5. The algorithm is
   1) Double center the data matrix $\mathbf{O}^2$ to obtain **B** (i.e., remove row and column means and add back in the grand mean of the squared data).
   2) Solve the singular value decomposition problem $B = ULU'$.
   3) Calculate $X = UL^{1/2}$.
6. This minimizes $\|B - XX'\|$.