Multivariate Verfahren

7.4. Multidimensional Scaling (MDS)

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based on slides by Sabine Hoffmann

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Sommersemester 2024

Introducion

- **What is MDS?** A technique for visualizing the similarity or dissimilarity of data points in a low-dimensional space.

- **Key Features:**

  Dimensionality Reduction: Transforms complex, high-dimensional data into a simpler, visually interpretable form (2D or 3D).

  Distance Preservation: Aims to retain the original distances between data points as accurately as possible.

- **Why Use MDS?** for data visualization and exploratory data analysis, It helps in understanding patterns and relationships in data.

The basic idea of MDS

- **Given**
  1. a set of n objects
  2. the distances/dissimilarities d_{ij} between them

- **We want to find** points in a lower dimensional space whose distances δ_{ij} are as close as possible to the d_{ij}.

- If all distances of the original objects are quantitative in nature, this in endeavour is more straightforward, since their distances are easily measured by **a metric** such as the euclidean distance $\longrightarrow$ *metric MDS*

- In other cases (quantitative distances), one needs to resort to more general dissimilarity measures to get the d_{ij}s $\longrightarrow$ *non-metric MDS*

Metric MDS

Metric MDS

The metric MDS goes back to Torgerson (1952, 1958) and can be divided into two models.

- distance model The objects $a_1, \ldots, a_n$ are transformed into distances $d_{i\ell},\ i, \ell = 1, \ldots, n$.

- spatial model The objects are represented by n points $\mathbf{y}_1, \ldots, \mathbf{y}_n$ in r-dimensional space in such a way that the metric distances $d_p(i, \ell) = d_p(\mathbf{y}_i, \mathbf{y}_\ell)$ of the objects approximate the distances $d_{i\ell}$ specified by the distance model as closely as possible.

Formal formulation of the problem

- Let $\mathbf{D} = (d_{i\ell})$ denote the matrix of original element-wise distances $d_{i\ell}$ and $\mathbf{\Delta} = (\delta_p(\mathbf{y}_i, \mathbf{y}_\ell))$ denote the corresponding matrix of element-wise distances for a lower-dimensional representation $\mathbf{Y} = (\mathbf{y}_1^\top, \ldots, , \mathbf{y}_n^\top)^\top \in \mathbf{R}^{nxr}$.

- We are looking for representation $\mathbf{Y}$ that minimizes the *cost or STRESS function*

$$\sum_{i \neq j} (d_{ij} - \delta_{ij})^2 \ .$$

- Clearly, this issue is **not unique**, because we could shift all points by a constant and obtain the same difference.

$\longrightarrow$ It can be is useful to assume centered points around the origin.

Classical metric MDS (cMDS)

- The starting point is the matrix of squared Euclidean distances with elements

$$d_2(i,\ell) = d_2(\mathbf{y}_i, \mathbf{y}_\ell) = (\mathbf{y}_i - \mathbf{y}_\ell)^\top (\mathbf{y}_i - \mathbf{y}_\ell), \quad i,\ell = 1,\ldots,n\,.$$

- Instead of finding $\mathbf{Y}$, we can focus on finding the following matrix

$$B = \boldsymbol{Y}\boldsymbol{Y}^T$$

- for which it holds that

$$d_{i\ell}^2 \quad = \quad b_{ii} + b_{\ell\ell} - 2b_{i\ell}\,.$$

Centering the distances first

- If we want to assume centering around the origin, which is the typical approach, we need to start with centering our distance matrix!

- For that, we use a centering matrix:

$$\mathbf{H} = \mathbf{I}_n - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^\top.$$

Note: we could replace $\frac{1}{n}$ with weights w_i, $\sum_{i=1}^n w_i = 1$ indicating the importance of each row of distances. Then, we would have $H = \mathbf{I}_n - \mathbf{1}_n(w_1, \ldots, w_n)^\top$.

- Then, we continue with

$$B = -\frac{1}{2}\boldsymbol{H}D\boldsymbol{H}.$$

Eigenvalue decomposition in MDS

Either way, we consider the eigenvalue decomposition of the matrix $\mathbf{B}$:

$$\mathbf{B} = \mathbf{P}\mathbf{\Lambda}\mathbf{P}^\top,$$

where

- $\boldsymbol{P}$ is the matrix of the orthonormalized eigenvectors of $\mathbf{B}$ and
- $\mathbf{\Lambda}$ is the diagonal matrix of the eigenvalues of $\mathbf{B}$ ordered by size.

Calculating the new representation in MDS

If one defines the eigenvectors for the r positive eigenvalues of $\mathbf{B}$ $\mathbf{y}_1 = \sqrt{\lambda_1}\,\mathbf{p}_1, \ldots, \mathbf{y}_r = \sqrt{\lambda_r}\,\mathbf{p}_r$ and the matrix

$$\mathbf{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_r)\,,$$

it holds that:

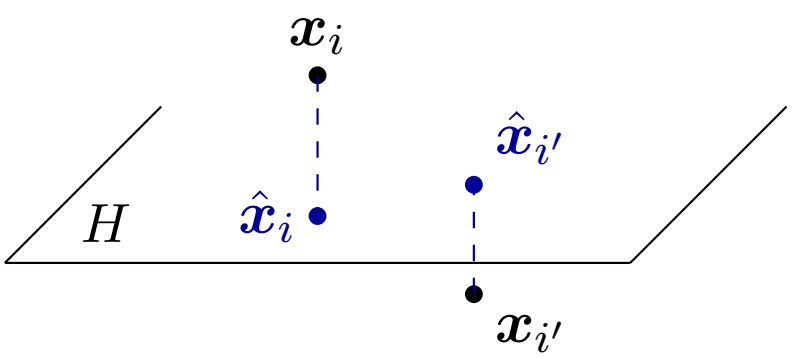
$$\mathbf{B} = \mathbf{P}\boldsymbol{\Lambda}^{\frac{1}{2}}\boldsymbol{\Lambda}^{\frac{1}{2}}\mathbf{P} = \mathbf{Y}\mathbf{Y}^\top\,.$$

$\rightarrow$ $\mathbf{Y} = (\mathbf{y}_1^\top, \ldots, , \mathbf{y}_n^\top)^\top$ is a representation of the objects and the lines of $\mathbf{Y}$ correspond to the coordinates.

Note

Classical MDS (i.e. MDS using the euclidean distance) yields the same results as PCA, see also Applied multivariate statistics. *However, MDS can also meaningfully be applied to distance matrices not generated under Euclidean distance measure where this no longer holds.*

Equivalence of cMDS and PCA

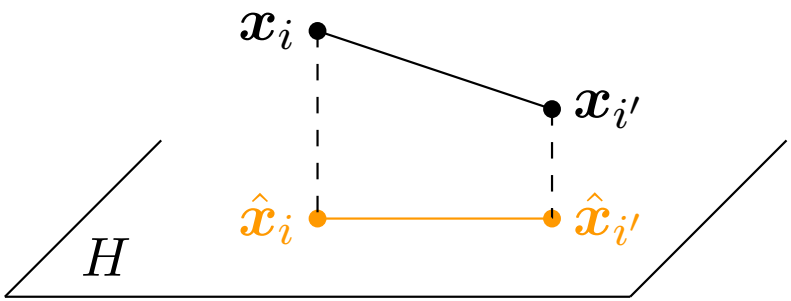


- **PCA:** Projection of the observations onto a subspace so that the maximum variance is retained

- Maximize

$$\boldsymbol{a}_p^\top \boldsymbol{S} \boldsymbol{a}_p\,, \quad p = 1, \ldots, m\,.$$

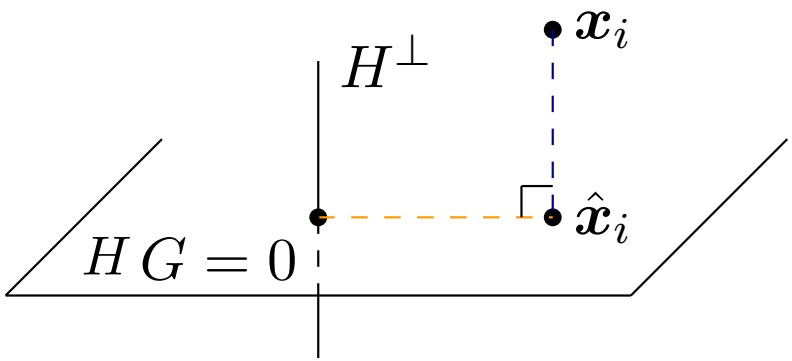
Equivalence of cMDS and PCA



- **MDS:** Find a subspace so that the original distances are preserved by the projection if possible $d\left(\hat{\boldsymbol{x}}_i, \hat{\boldsymbol{x}}_{i'}\right)$
- Minimize

$$\sum_{i \neq i'} \left(d\left(\hat{\boldsymbol{x}}_i, \hat{\boldsymbol{x}}_{i'}\right) - d\left(\boldsymbol{x}_i, \boldsymbol{x}_{i'}\right)\right)^2$$

Equivalence of cMDS and PCA



- Explained variance (by H):

$$I(H) = \frac{1}{n}\sum_{i=1}^{n} \|\hat{\boldsymbol{x}}_i\|^2$$

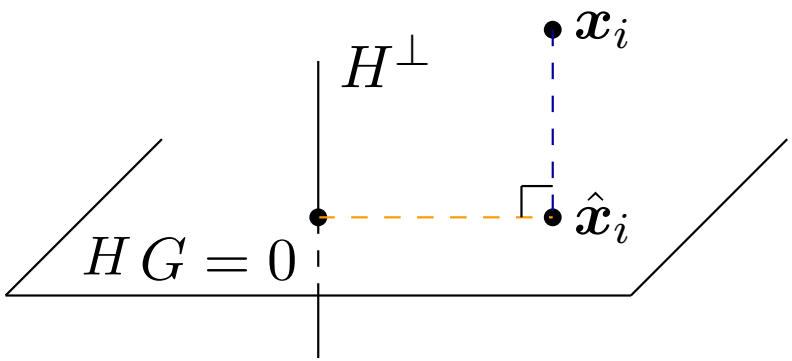
- Residual variance:

$$I(H^\perp) = \frac{1}{n}\sum_{i=1}^{n} \|\boldsymbol{x}_i - \hat{\boldsymbol{x}}_i\|^2$$

- Total variance:

$$I_G = I_0 = \frac{1}{n}\sum_{i=1}^{n} \|\boldsymbol{x}_i\|^2$$

Equivalence of cMDS and PCA



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- Residual variance:

$$I(H^\perp) = \frac{1}{n}\sum_{i=1}^{n} \|\boldsymbol{x}_i - \hat{\boldsymbol{x}}_i\|^2$$

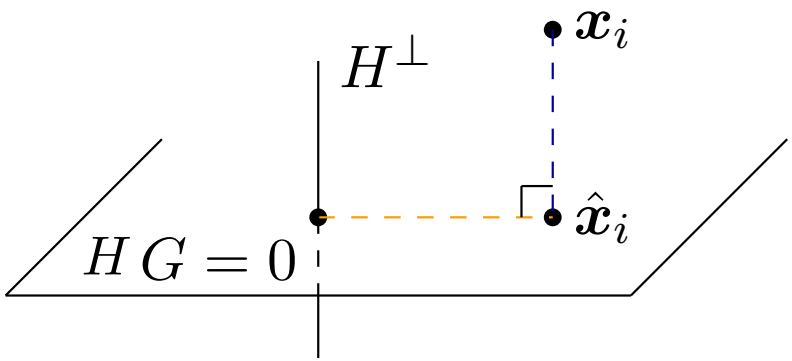
- According to Pythagoras' theorem:
  $\|\boldsymbol{x}_i\|^2 = \|\hat{\boldsymbol{x}}_i\|^2 + \|\boldsymbol{x}_i - \hat{\boldsymbol{x}}_i\|^2$

- Total variance:

$$I_G = I_0 = \frac{1}{n}\sum_{i=1}^{n} \|\boldsymbol{x}_i\|^2$$

- Total variance = explained variance + residual variance

Equivalence of cMDS and PCA



- Explained variance (by H):

$$I(H) = \frac{1}{n}\sum_{i=1}^{n} \|\hat{\boldsymbol{x}}_i\|^2$$

- Residual variance:

$$I(H^\perp) = \frac{1}{n}\sum_{i=1}^{n} \|\boldsymbol{x}_i - \hat{\boldsymbol{x}}_i\|^2$$

$\Rightarrow$ Minimizing the distance criterion and maximizing the variance criterion leads to the same result for the euclidean distance!

- Total variance:

$$I_G = I_0 = \frac{1}{n}\sum_{i=1}^{n} \|\boldsymbol{x}_i\|^2$$

Summary of cMDS

Goal: Determine a lower-dimensional representation from a distance matrix D

1. Calculate the centering matrix $H = \mathbf{I}_n - \mathbf{1}_n(w_1, \ldots, w_n)^\top$ (mostly, $w_i = \frac{1}{n}$).

2. Determine, for $\boldsymbol{D}$ denoting the matrix of squared euclidean distances

$$B = -\frac{1}{2}\boldsymbol{HDH}.$$

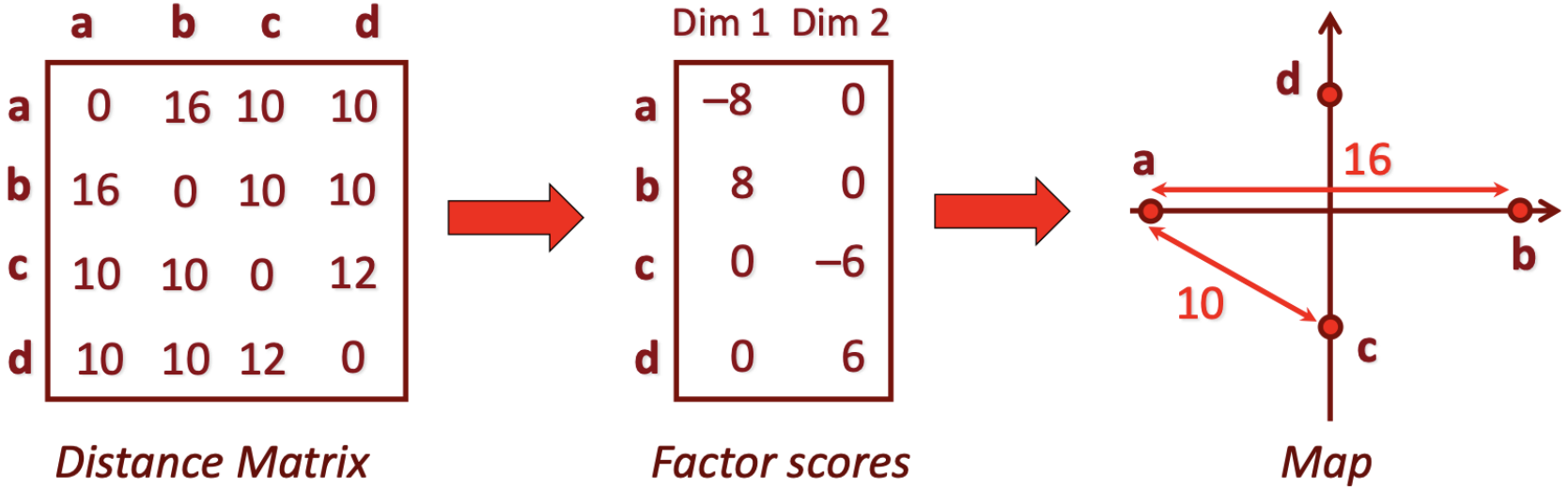
3. Carry out a spectral decomposition of B:

$$B = P\Lambda P^T$$

4. Calculate the points in the lower dimensional representation $\mathbf{Y}$.

Small hands-on example of cMDS I

Figure 1: The Main Steps of Multidimensional Scaling: 1) Start with a distance matrix, 2) Transforms the distance matrix into a set of factor scores, and 3) Plot the observations using their factor scores. Here the distances on the map exactly recover the distances in the original matrix.



Source:https://personal.utdallas.edu/~herve/abdi-MDS-sage2022.pdf

Small hands-on example of cMDS II

Here, we have

$$\mathbf{D}_{\text{Euclid}} = \begin{bmatrix} 0 & 16 & 10 & 10 \\ 16 & 0 & 10 & 10 \\ 10 & 10 & 0 & 12 \\ 10 & 10 & 12 & 0 \end{bmatrix}, \mathbf{D} = \begin{bmatrix} 0 & 256 & 100 & 100 \\ 256 & 0 & 100 & 100 \\ 100 & 100 & 0 & 144 \\ 100 & 100 & 144 & 0 \end{bmatrix}$$

and a "weights vector"

$$\mathbf{w}^\top = \begin{bmatrix} .25 & .25 & .25 & .25 \end{bmatrix}.$$

This results in the following centering matrix:

$$\boldsymbol{H} = \begin{bmatrix} .75 & -.25 & -.25 & -.25 \\ -.25 & .75 & -.25 & -.25 \\ -.15 & -.25 & .75 & -.25 \\ -.25 & -.25 & -.25 & .75 \end{bmatrix}.$$

Small hands-on example of cMDS III

Next, we calculate

$$B = -\frac{1}{2}\boldsymbol{HDH} = \begin{bmatrix} 64 & -64 & 0 & 0 \\ -64 & 64 & 0 & 0 \\ 0 & 0 & 36 & -36 \\ 0 & 0 & -36 & 36 \end{bmatrix}$$

The eigen-decomposition of B gives

$$B = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top \text{ with } \quad \mathbf{U} = \begin{bmatrix} -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \text{ and } \boldsymbol{\Lambda} = \begin{bmatrix} 128 & 0 \\ 0 & 72 \end{bmatrix}.$$

Small hands-on example of cMDS IV

Which gives us the following lower-dimensional representation:

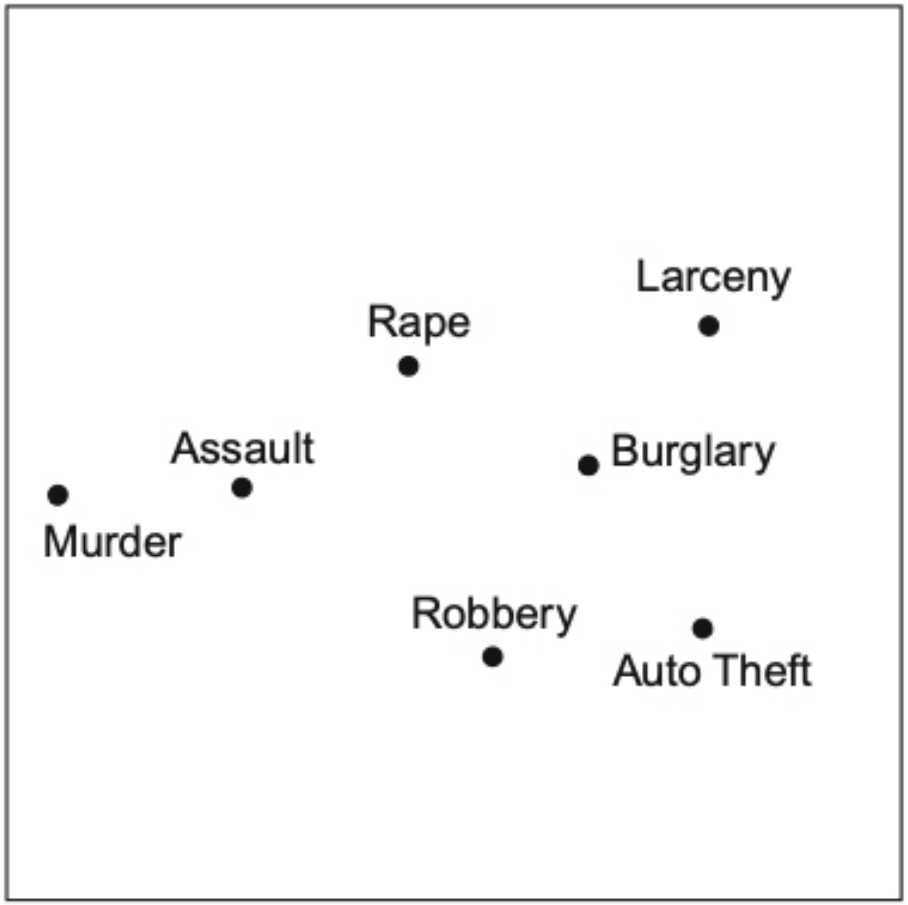
$$\mathbf{Y} = \mathbf{U}\mathbf{\Lambda}^{\frac{1}{2}} = \begin{bmatrix} -\sqrt{\frac{128}{2}} & 0 \\ \sqrt{\frac{128}{2}} & 0 \\ 0 & -\sqrt{\frac{72}{2}} \\ 0 & \sqrt{\frac{72}{2}} \end{bmatrix} = \begin{bmatrix} -\sqrt{64} & 0 \\ \sqrt{64} & 0 \\ 0 & -\sqrt{36} \\ 0 & \sqrt{36} \end{bmatrix}$$

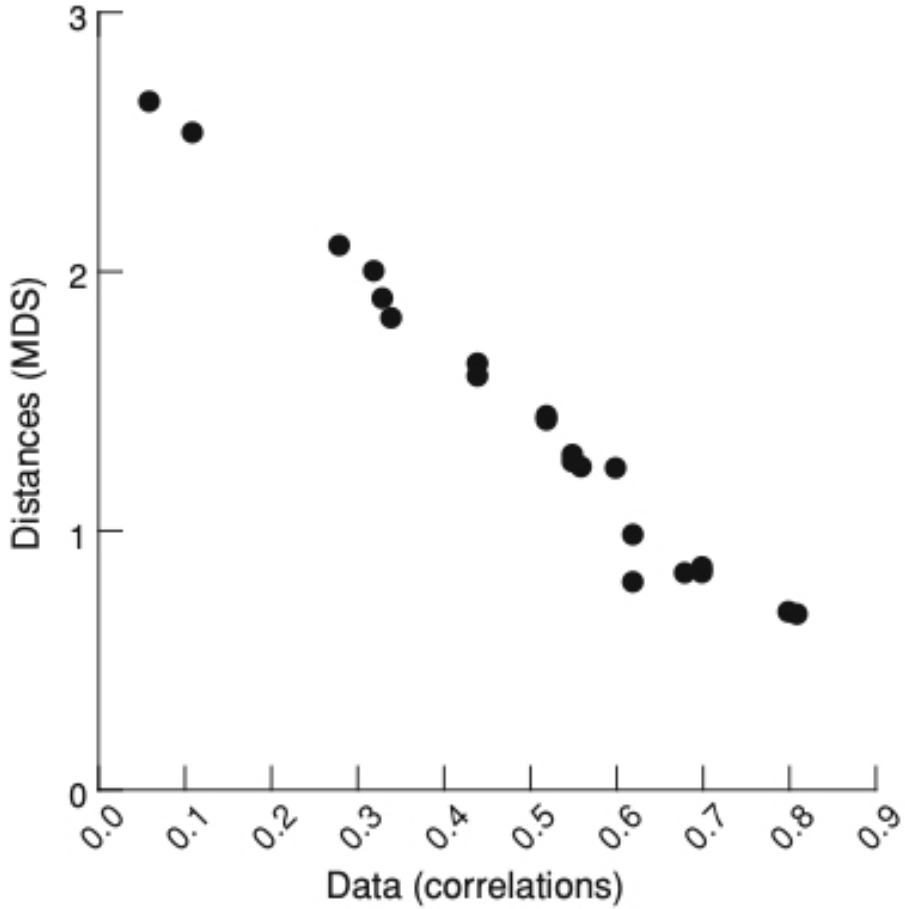
$$= \begin{bmatrix} -8 & 0 \\ 8 & 0 \\ 0 & -6 \\ 0 & 6 \end{bmatrix}.$$

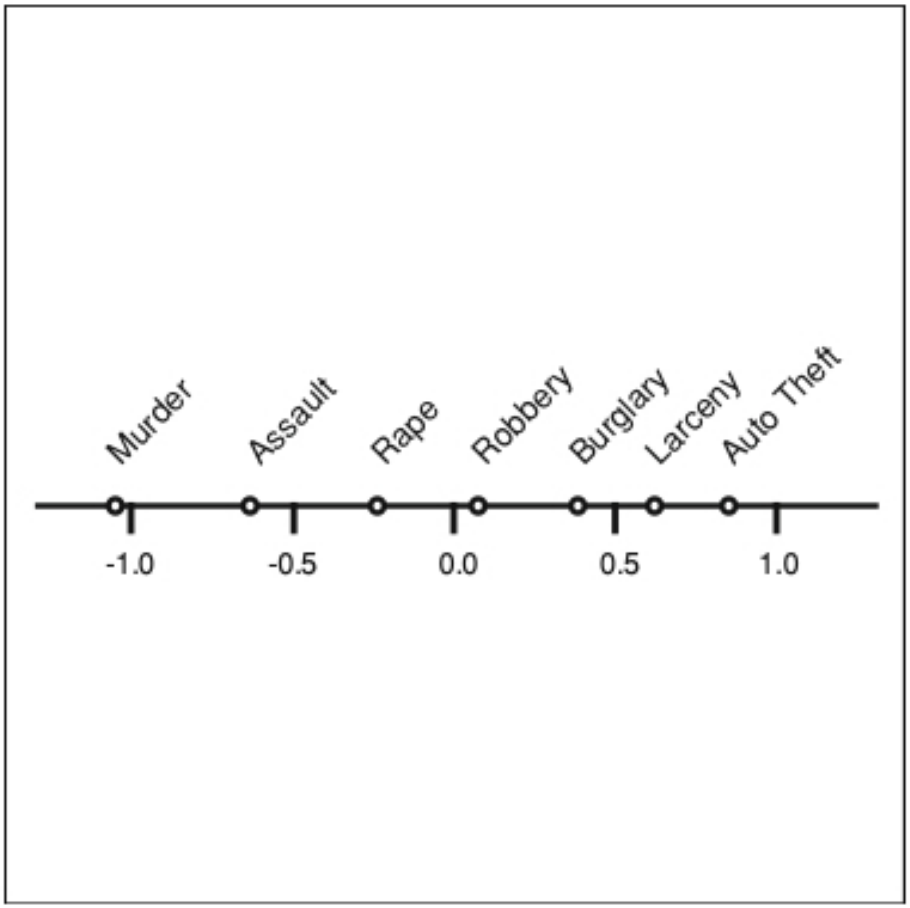
Applied example: Criminality in the US

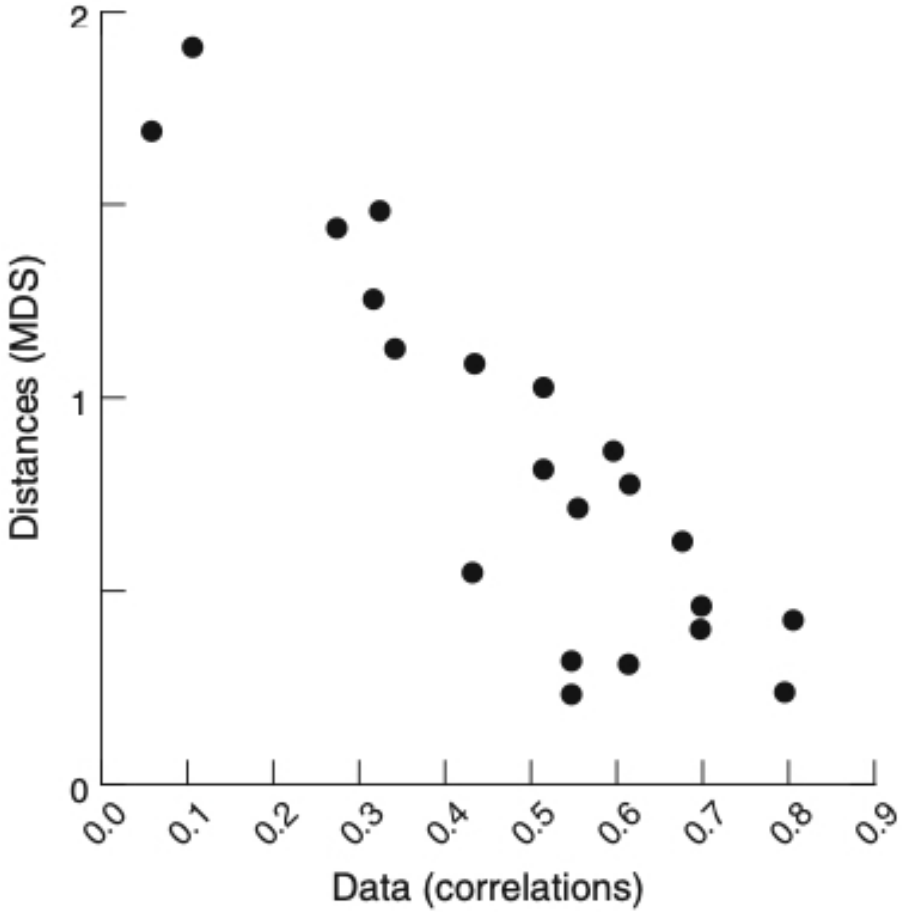
Table 1.1 Correlations of crime rates over 50 U.S. states

Crime	Murder	Rape	Robbery	Assault	Burglary	Larceny	Auto theft
Murder	1.00	0.52	0.34	0.81	0.28	0.06	0.11
Rape	0.52	1.00	0.55	0.70	0.68	0.60	0.44
Robbery	0.34	0.55	1.00	0.56	0.62	0.44	0.62
Assault	0.81	0.70	0.56	1.00	0.52	0.32	0.33
Burglary	0.28	0.68	0.62	0.52	1.00	0.80	0.70
Larceny	0.06	0.60	0.44	0.32	0.80	1.00	0.55
Auto theft	0.11	0.44	0.62	0.33	0.70	0.55	1.00


Larceny
Rape
Assault
Burglary
Murder
Robbery
Auto Theft


Distances (MDS)
Data (correlations)
0
1
2
3
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9


Murder
Assault
Rape
Robbery
Burglary
Larceny
Auto Theft
-1.0
-0.5
0.0
0.5
1.0


Distances (MDS)
Data (correlations)
0
1
2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9

Iterative approach to solutions

Especially not performing classical MDS, a typical solution is to iteratively solve the minimization of the *cost or STRESS* function by

1. Initializing a random lower-dimensional representation $\mathbf{Y}$
2. Improving on it until the STRESS function is smaller some constant c.

The improvement can be carried out via isotonic (or monotonic) regression, the technique of fitting a free-form line to a sequence of observations, *especially for non-metric MDS*.

Non-metric MDS

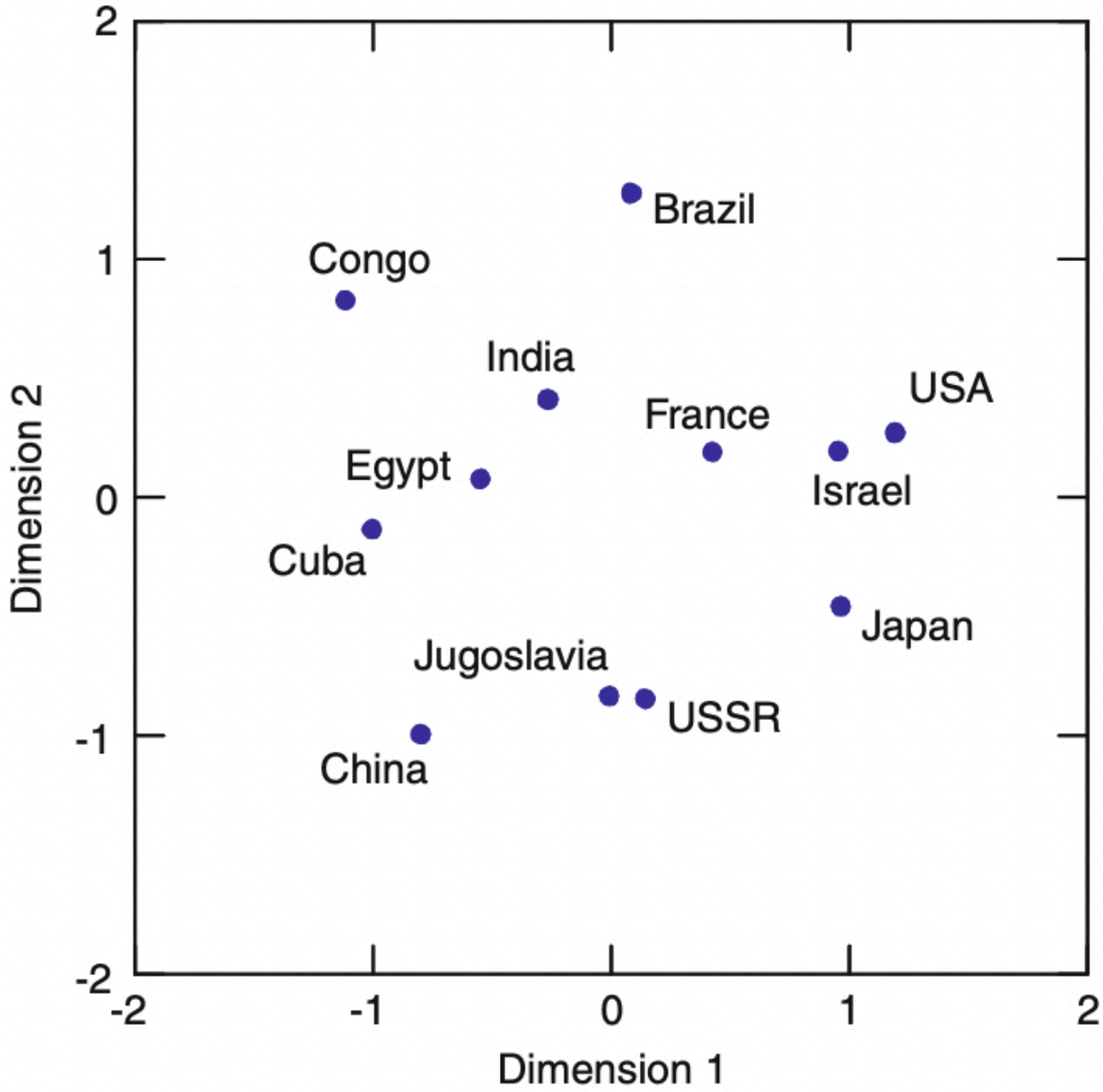
Nichtmetrische MDS

Non-metric MDS methods go back to Shepard (1962) and only assume that there is a *monotonic* relationship between the similarity ranking of the object pairs and the object distances.

The monotonicity condition is as follows:

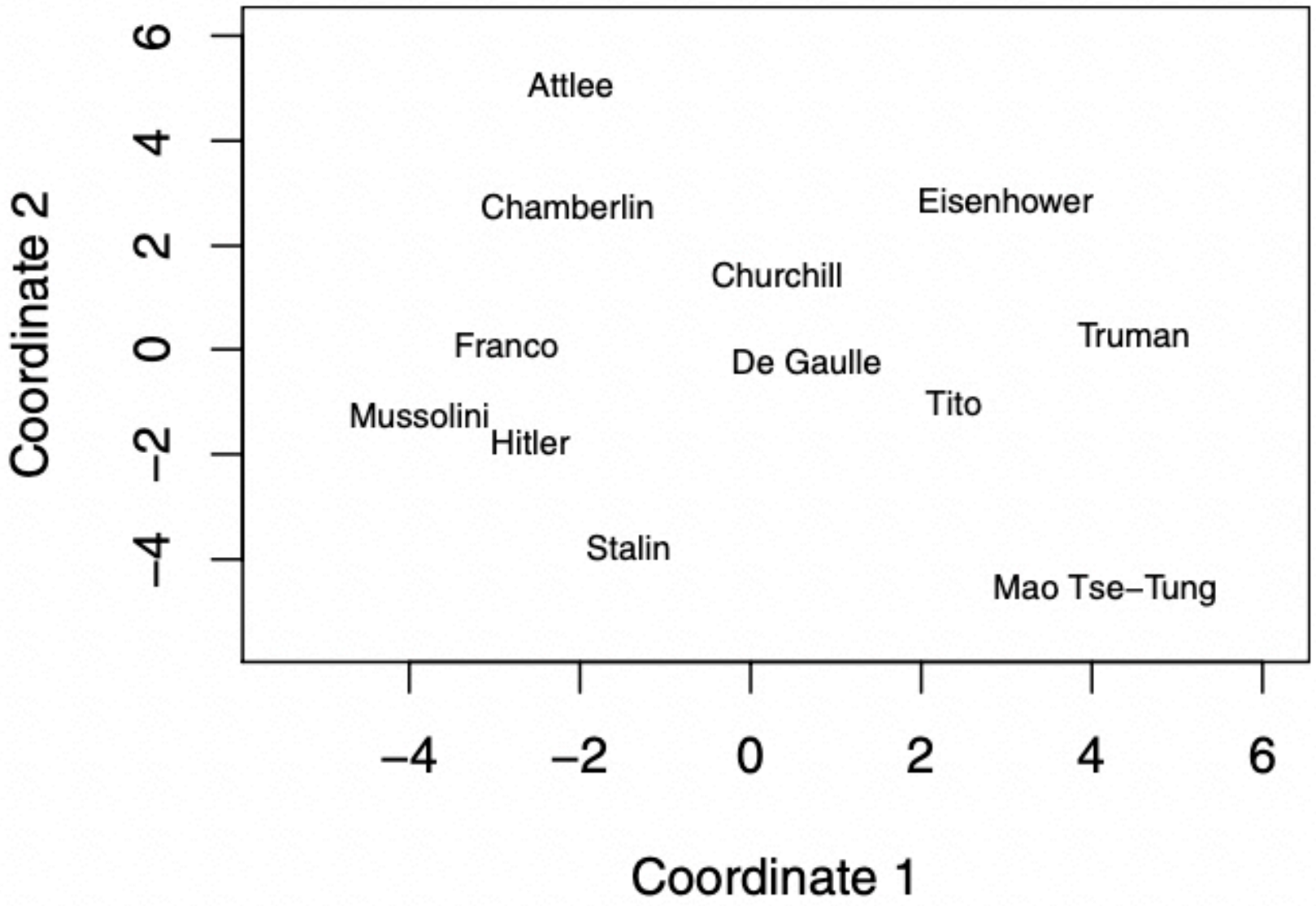
$$(i, \tilde{i}) \text{ more similar than } (k, \tilde{k}) \;\Rightarrow\; d_{i\tilde{i}} \;<\; d_{k\tilde{k}}$$

Country		1	2	3	4	5	6	7	8	9	10	11	
Brazil	1	–											
Congo	2	4.83	–										
Cuba	3	5.28	4.56	–									
Egypt	4	3.44	5.00	5.17	–								
France	5	4.72	4.00	4.11	4.78	–							
India	6	4.50	4.83	4.00	5.83	3.44	–						
Israel	7	3.83	3.33	3.61	4.67	4.00	4.11	–					
Japan	8	3.50	3.39	2.94	3.83	4.22	4.50	4.83	–				
China	9	2.39	4.00	5.50	4.39	3.67	4.11	3.00	4.17	–			
USSR	10	3.06	3.39	5.44	4.39	5.06	4.50	4.17	4.61	5.72	–		
USA	11	5.39	2.39	3.17	3.33	5.94	4.28	5.94	6.06	2.56	5.00	–	
Jugoslavia	12	3.17	3.50	5.11	4.28	4.72	4.00	4.44	4.28	5.06	6.67	3.56	–


Brazil
Congo
India
USA
France
Egypt
Israel
Cuba
Japan
Jugoslavia
USSR
China
Dimension 2
Dimension 1
2
1
0
-1
-2
-2
-1
0
1
2

	Htl	Mss	Chr	Esn	Stl	Att	Frn	DGl	MT-	Trm	Chm	Tit
Hitler	0											
Mussolini	3	0										
Churchill	4	6	0									
Eisenhower	7	8	4	0								
Stalin	3	5	6	8	0							
Attlee	8	9	3	9	8	0						
Franco	3	2	5	7	6	7	0					
De Gaulle	4	4	3	5	6	5	4	0				

	Htl	Mss	Chr	Esn	Stl	Att	Frn	DGl	MT-	Trm	Chm	Tit
Mao Tse-Tung	8	9	8	9	6	9	8	7	0			
Truman	9	9	5	4	7	8	8	4	4	0		
Chamberlin	4	5	5	4	7	2	2	5	9	5	0	
Tito	7	8	2	4	7	8	3	2	4	5	7	0


Attlee
Chamberlin
Eisenhower
Churchill
Truman
Franco
De Gaulle
Tito
Mussolini
Hitler
Stalin
Mao Tse–Tung
Coordinate 2
6
4
2
0
−2
−4
−4
−2
0
2
4
6
Coordinate 1

Solution of non-metric MDS

The aim is to determine a representation of the objects that fulfills the monotonicity condition in a space with the smallest possible dimensions.

Iteratively minimize the following STRESS function:

$$S(\mathbf{Y}) = \sqrt{\frac{\sum_{k<\ell} (d_{k\ell} - \hat{d}_{k\ell})^2}{\sum_{k<\ell} d_{k\ell}^2}}\,.$$

$\rightarrow$ The most widely used method is that of Kruskal (1964).

Cool visualization

A really nice interactive visualization of MDS is given in the following blog-post:

Visualizing MNIST: An Exploration of Dimensionality Reduction