Multidimensional Scaling and Distance Embedding

Main Idea

Classical Multidimensional Scaling

Non-metric Multidimensional Scaling

Lecture 13
Multidimensional Scaling and Distance Embedding

Reading: Izenman Chapter 13

The main reference for these slides is from Dr. Markus Kalisch's Lecture Notes at https://stat.ethz.ch/education/semesters/ss2012/ams/slides/v4.1.pdf

DSA 8070 Multivariate Analysis

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Notes

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Agenda

1. Main Idea
2. Classical Multidimensional Scaling
3. Non-metric Multidimensional Scaling

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Principal Component Analysis and Multidimensional Scaling

- Principal Component Analysis (PCA):

  In PCA, one starts with n data points $\boldsymbol{y}_i \in \mathbb{R}^p$, then tries to find a low-dimensional projection of these points, e.g., $\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n \in \mathbb{R}^r$ with $r < p$, in such a way as to maximize the variance (thus minimizing the reconstruction error)

- Multidimensional Scaling (MDS):

  In MDS, instead of being given the data $\boldsymbol{Y} = \{\boldsymbol{y}_i\}_{i=1}^n$, a matrix of distances or dissimilarities between the data points, $\boldsymbol{D} = \{d_{ij}\}_{i,j=1}^n$ is provided. The goal of MDS is to find a set of points in a low-dimensional Euclidean space $\mathbb{R}^r$, usually $r = 2$, whose inter-point distances are as close as possible to the $\{d_{ij}\}$ distances

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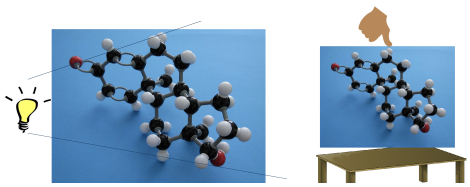
Basic Idea of MDS

Represent a high-dimensional point cloud in a low (usually 2)-dimensional Euclidean space while *preserving, as closely as possible, the inter-point distances*. Commonly used MDS methods include classical/metric MDS and non-metric MDS:

- Classical/Metric MDS: Use a clever projection
- Non-metric MDS: Squeeze data on table



Source: Dr. Markus Kalisch's Lecture Notes on MDS

Notes

Classical MDS (cMDS)

- **Goal**: Given pairwise distances among points, recover the position of the points!
- **Example**: Distance between 10 US major cities

```
> UScitiesD
```

	Atlanta	Chicago	Denver	Houston	LosAngeles	Miami	NewYork	SanFrancisco	Seattle
Chicago	587								
Denver	1212	920							
Houston	701	940	879						
LosAngeles	1936	1745	831	1374					
Miami	604	1188	1726	968	2339				
NewYork	748	713	1631	1420	2451	1092			
SanFrancisco	2139	1858	949	1645	347	2594	2571		
Seattle	2182	1737	1021	1891	959	2734	2408	678	
Washington.DC	543	597	1494	1220	2300	923	205	2442	2329

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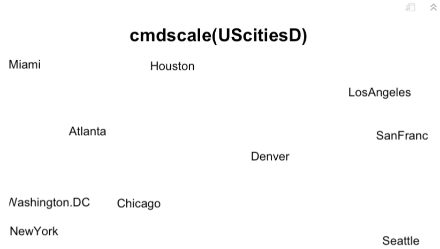
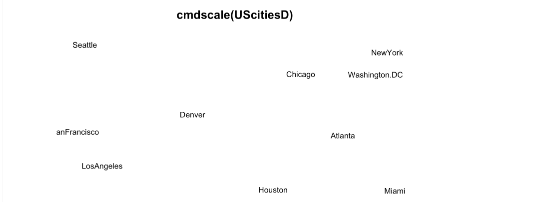
Classical MDS: First Try

```
loc <- cmdscale(UScitiesD)
x <- loc[, 1]; y <- loc[, 2]
plot(x, y, type = "n", xlab = "", ylab = "", asp = 1,
     axes = FALSE, main = "cmdscale(UScitiesD)")
text(x, y, rownames(loc), cex = 0.8)
```
```








Notes
```

Classical MDS: Flip Axes


```
# Flip Axes
x1 <- -loc[, 1]; y1 <- -loc[, 2]
plot(x1, y1, type = "n", xlab = "", ylab = "", asp = 1,
     axes = FALSE, main = "cmdscale(UScitiesD)")
text(x1, y1, rownames(loc), cex = 0.8)
'''
```



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Another Example: Air Pollution in US Cities

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```
> summary(dat)
      SO2              temp            manu            popul       
 Min.   :  8.00   Min.   :43.50   Min.   :  35.0   Min.   :  71.0  
 1st Qu.: 13.00   1st Qu.:50.60   1st Qu.: 181.0   1st Qu.: 299.0  
 Median : 26.00   Median :54.60   Median : 347.0   Median : 515.0  
 Mean   : 30.05   Mean   :55.76   Mean   : 463.1   Mean   : 608.6  
 3rd Qu.: 35.00   3rd Qu.:59.30   3rd Qu.: 462.0   3rd Qu.: 717.0  
 Max.   :110.00   Max.   :75.50   Max.   :3344.0   Max.   :3369.0  
      wind            precip         predays     
 Min.   : 6.000   Min.   : 7.05   Min.   : 36.0  
 1st Qu.: 8.700   1st Qu.:30.96   1st Qu.:103.0  
 Median : 9.300   Median :38.74   Median :115.0  
 Mean   : 9.444   Mean   :36.77   Mean   :113.9  
 3rd Qu.:10.600   3rd Qu.:43.11   3rd Qu.:128.0  
 Max.   :12.700   Max.   :59.80   Max.   :166.0  
```

- Range of `manu` and `popul` is much bigger than range of `wind`
- Need to standardize to give every variable equal weight

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Air Pollution in US Cities Example

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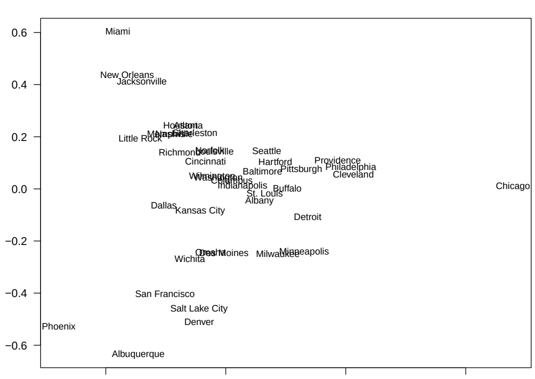

Notes

Classical MDS: Technical Details

- **Input**: $D = \{d_{ij}\}_{i,j=1}^{n}$, the Euclidean distances between n objects in p dimensions
- **Output**: $\boldsymbol{X} = \{\boldsymbol{x}_i\}_{i=1}^{n}$, the "position" of points up to rotation, reflection, shift
- Two steps:
  - Compute inner products matrix $\boldsymbol{B} = \boldsymbol{X}\boldsymbol{X}^T$ from distance

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

  - Perform spectral decomposition to compute positions from $\boldsymbol{B}$ (see next slide)

Notes

Classical MDS: Technical Details

- Since $\boldsymbol{B} = \boldsymbol{X}\boldsymbol{X}^T$, we need the "square root" of $\boldsymbol{B}$
- Since $\boldsymbol{B}$ is a symmetric and positive definite $n \times n$ matrix $\Rightarrow$ $\boldsymbol{B}$ can be diagonalized:

$$\boldsymbol{B} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$$

  Λ is a diagnoal matrix with $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ on diagonal
- Assuming the rank of $\boldsymbol{B} = p$, so that the last $n-p$ of its eigenvalues will be zero $\Rightarrow$ $\boldsymbol{B}$ can be written as

$$\boldsymbol{B} = \boldsymbol{V}_1\Lambda_1\boldsymbol{V}_1^T,$$

  where $\boldsymbol{V}_1$ contains the first p eigenvectors and Λ_1 the p non-zero eigenvalues. Take "square root": $\boldsymbol{X} = \boldsymbol{V}_1\boldsymbol{\Lambda}_1^{-\frac{1}{2}}$

Notes

Classical MDS: Low-Dimensional Representation

- Keep only few (e.g. 2) largest eigenvalues and corresponding eigenvectors
- The resulting $\boldsymbol{X}$ will be the low-dimensional representation we were looking for
- "Goodness of fit" (GOF) if we reduce to r dimensions:

$$\text{GOF} = \frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{n} \lambda_i}$$

- Finds "optimal" low-dim representation:

$$\text{Find } \boldsymbol{x}_1, \cdots, \boldsymbol{x}_n \in \mathbb{R}^r$$

$$\text{to minimize } \sum_{i=1}^{n}\sum_{j=1}^{n}(d_{ij} - d(\boldsymbol{x}_i, \boldsymbol{x}_j))^2$$

Notes

Classical MDS: Pros and Cons

- + Optimal for Euclidean input data
- + Still optimal, if $\boldsymbol{B}$ has non-negative eigenvalues
- + Very fast to compute
- - There is no guarantee it will be optimal if $\boldsymbol{B}$ has negative eigenvalues

Notes

Non-metric MDS: Idea

- Sometimes, there is no well-defined metric on original points
- Absolute values are not as meaningful, but the ranking is important, for example, in ordinal data and survey data (subjective preferences)
- Non-metric MDS finds a low-dimensional representation, which respects the ranking of distances

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Non-metric MDS: Theory

- δ_{ij} is the true dissimilarity, d_{ij} is the distance of representation
- Minimize STRESS:

$$S = \frac{\sum_{i<j} (\theta(\delta_{ij}) - d_{ij})^2}{\sum_{i<j} d_{ij}^2},$$

  where $\theta(\cdot)$ is an increasing function
- Optimize over both position of points and θ
- $\hat{d}_{ij} = \theta(\delta_{ij})$ is called "disparity"
- Solved numerically (isotonic regression); Classical MDS as starting value; very time consuming

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Non-metric MDS: Pros andn Cons

- +: Fulfills a clear objective (minimize `STRESS`) without many assumptions
- +: Results don't change with rescaling or monotonic variable transformation
- +: Works even if you only have rank information
- -: computation can be slow in "large" problems
- -: Usually only local (not global) optimum found
- -: Only gets ranks of distances right

Notes

House of Representatives Voting Data

Romesburg (1984) gives a set of data that shows the number of times 15 congressmen from New Jersey voted differently in the House of Representatives on 19 environmental bills

```
> voting[1:6, 1:6]
                 Hunt(R) Sandman(R) Howard(D) Thompson(D) Freylinghuysen(R) Forsythe(R)
Hunt(R)                0          8        15          15                10           9
Sandman(R)             8          0        17          12                13          13
Howard(D)             15         17         0           9                16          12
Thompson(D)           15         12         9           0                14          12
Freylinghuysen(R)     10         13        16          14                 0           8
Forsythe(R)            9         13        12          12                 8           0
```

Question: Do people in the same party vote alike?

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Kruskal's Non-metric Multidimensional Scaling in R

Usage

```
isoMDS(d, y = cmdscale(d, k), k = 2, maxit
= 50, trace = TRUE, tol = 1e-3, p = 2)
```

Voting Example

```
library(MASS)
voting_mds <- isoMDS(voting, k = 2)
str(voting_mds)
par(las = 1, mar = c(2, 2, 0.5, 0.5))
plot(voting_mds$points, type = "n", xlim = c(-12, 8),
     xlab = "", ylab = "")
text(voting_mds$points, labels = rownames(voting_mds$points),
     cex = 0.7, col = col)
```

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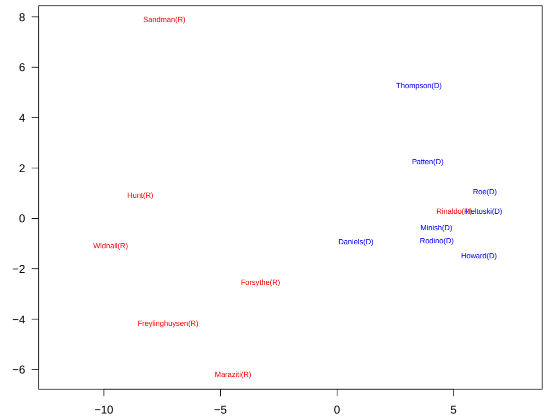
Non-metric MDS: Voting Example



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Summary

- Classical MDS:
  - Finds low-dim projection that respects distances
  - Optimal for euclidean distances
  - No clear guarantees for other distances
  - Fast to compute (can use `cmdscale` in `R`)
- Non-metric MDS:
  - Squeezes data points on table
  - Respects only rankings of distances
  - (Locally) solves clear objective
  - Computation can be slow (can use `isoMDS` from the `R` package “`MASS`”)

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