Lecture 14
Multidimensional Scaling

DSA 8070 Multivariate Analysis
November 15- November 19, 2021

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Notes

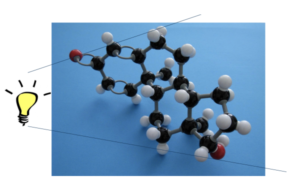
Agenda

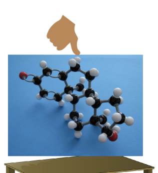
1. Main Idea
2. Classical Multidimensional Scaling
3. Non-metric Multidimensional Scaling

Notes

Basic Idea of Multidimensional Scaling (MDS)

- Represent high-dimensional point cloud in low (usually 2) dimensional Euclidean space while preserving as well as possible the inter-point distances
- 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

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

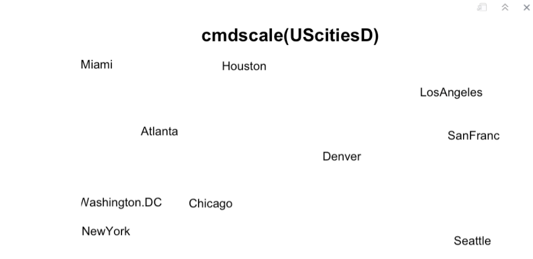
```
> UScitiesD
```

	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

Notes

Classical MDS: First Try

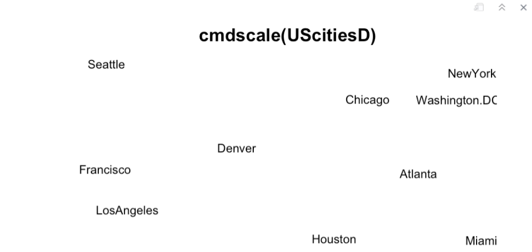

```
loc <- cmdscale(UScitiesD)
x <- loc[, 1]; y <- loc[, 2]
plot(x, y, type = "n", xlab = "", ylab = "", asp = 1,
     axes = FALSE, main = "cmdscale(UScitiesD)")
text(x, y, rownames(loc), cex = 0.8)
```



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)
```



Notes

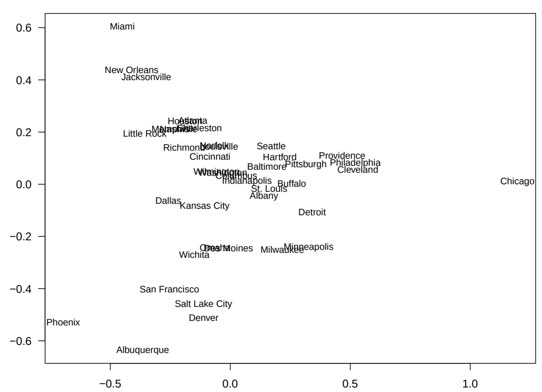
Another Example: Air Pollution in US Cities

```
> 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

Notes

Air Pollution in US Cities Example



Notes

Classical MDS: Technical Details

- **Input**: Euclidean distances between n objects in p dimensions
- **Output**: "Position" of points up to rotation, reflection, shift
- Two steps:
  - Compute inner products matrix $\boldsymbol{B}$ 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

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Main Idea
Classical Multidimensional Scaling
Non-metric Multidimensional Scaling

- 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 m dimensions:

$$\mathrm{GOF} = \frac{\sum_{i=1}^{m} \lambda_i}{\sum_{i=1}^{n} \lambda_i}$$

- Finds "optimal" low-dim representation: Minimizes

$$S = \sum_{i=1}^{n} \sum_{j=1}^{n} \left(d_{ij}^2 - (d_{ij}^m)^2\right)^2$$

Notes

Classical MDS: Pros and Cons

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- \+ 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 that meaningful, but the ranking is important
- Non-metric MDS finds a low-dimensional representation, which respects the ranking of distances

Notes

Non-metric MDS: Theory

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

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

  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

Notes

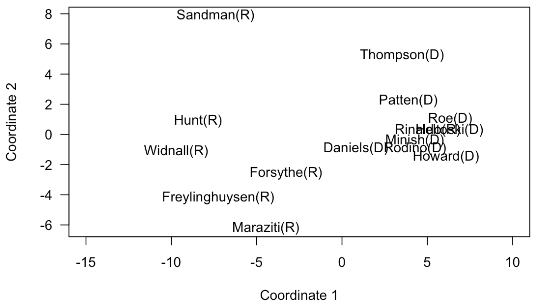
Non-metric MDS: Pros andn Cons

- +: Fulfills a clear objective (minimize $\texttt{STRESS}$) 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

Non-metric MDS: Voting Example

- Do people in the same party vote alike?
- Agreement of 15 congressman in 19 votes



Notes

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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