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## Data Analysis, Lecture 4: Data visualization: Feature selection & Linear methods

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# Data Analysis - Lecture 4

## Data visualization: Feature selection & Linear methods

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# Plan

- 1 Introduction
- 2 Feature selection methods
- 3 Linear Feature extraction methods
- 4 Bibliography

# Outline

- 1 Introduction
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# Definitions

## Visualization: Definition

Visualization is a branch of computer science involving the processing, analysis and graphical representation of data from diverse fields: social sciences, finance, medicine, entertainment, etc.

- One goal of visualization is to visually represent data that does not necessarily have a natural geometric interpretation.

Data visualization relies on two main fields:

- Statistics
- Computer graphics

# Definitions

It is important to distinguish between the areas of image processing, computer graphics and visualization.

## Image processing VS Computer graphics VS Visualization

- Image processing is the study of 2D images to extract information or to modify their characteristics.
- Computer graphics allows to create, draw and render images (2D or 3D), or videos of almost anything using a computer.
- Visualization allows the exploration of data represented in a visual form that helps our understanding of a shown phenomenon.

# Why visualizing data ?

- A better visualization leads to a better understanding.
- Graphical visualization is an efficient way to communicate information clearly and efficiently.
- A lot of data are high dimensional and difficult to grasp without a lower dimensionality projection.
- Many Machine Learning techniques can benefit from data visualization:
  - Regression and time series analysis: to visualize the data and guess the model
  - Clustering: To guess the number of clusters and their shape, or to detect anomalies/outliers.
  - Classification: To assess classes' separability.

# Why visualizing data ?

The number of features can be very large:

- Genomic data: thousands of variables
- Image data: a 64x64 image contains 4096 3D variables
- Text data: frequency of words or phrases in a web page
  - more than ten thousand features

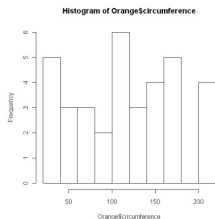


# When visualizing data ?

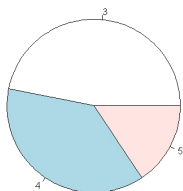
- When performing an exploratory task on new data.
- When the data are inhomogeneous or noisy.
- When the data are high dimensional and uneasy to grasp.
- To visualize and assess the result of a Machine Learning task in low dimension and see if it visually makes sense.
- To see if the data need to be transformed (rotation, dimension reduction, compression, etc.) before using a Machine Learning or data analysis task.

# Univariate data

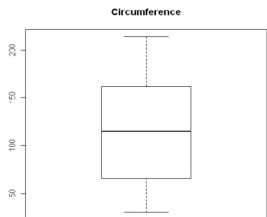
- Represents the distribution of a variable
- Represents categorical variable distribution
- Represents trends and error margins



(a) Histogram



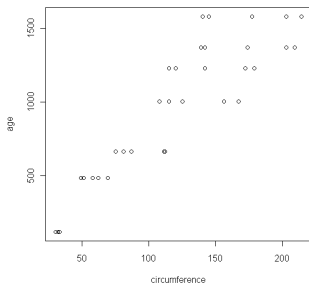
(b) Pie Plot  
(camembert)



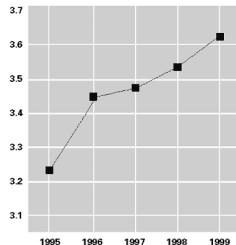
(c) Box plot (boîte à moustaches)

# Bivariate data (1/2)

- Representation, correlation analysis, trend analysis



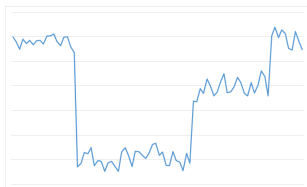
(d) Representation



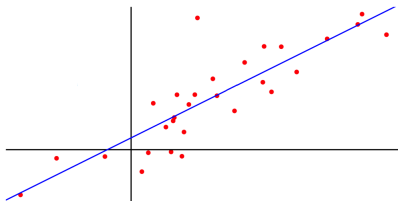
(e) Time series trends

# Bivariate data (2/2)

- Representation, correlation analysis, trend analysis

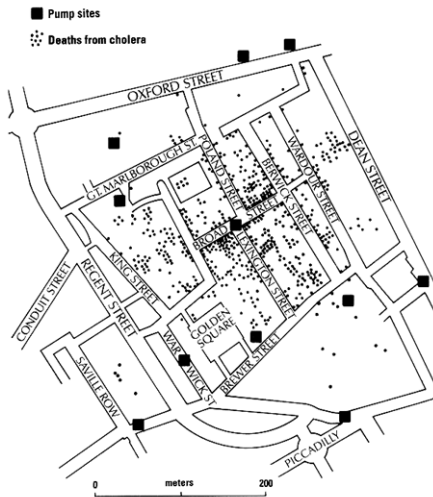


(f) Time series



(g) Correlation & Regression

# Cross-bivariate data



# Multivariate data

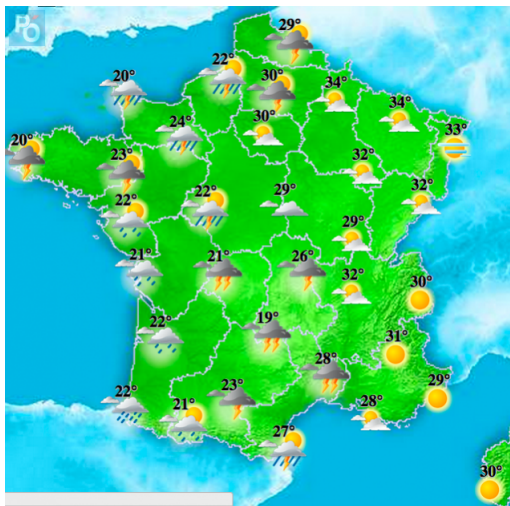
Representing multi-dimensional data in 2D (or 3D) is more complex but can help understand them.

## Multi-variate data visualization techniques

- Dimension reduction and/or projection on 2 variables
- Icon-based, text-based, or color-based representations for the missing dimensions.

# Multivariate data

Weather forecast: City coordinates (2 variables), weather, temperature.



# The curse of dimensionality

The “*curse of dimensionality*” is a term introduced in 1961 by Bellman referring to the problem of the explosive increase in data volume associated with adding extra dimensions in a mathematical space.

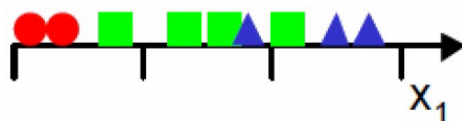
## Why the curse of dimensionality matters

- High dimensional data are difficult to efficiently visualize in 2D without losing meaningful information.
  - While computer algorithms can grasp information in higher dimensional spaces than humans, past some point, they too have trouble extracting the meaningful information.
- 
- We will illustrate this problem with a simple example.



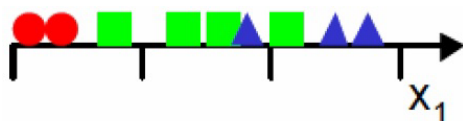
# The Toy problem

We consider a Pattern Recognition problem with 3 classes. We have 9 available observations represented in 1 dimension.



# The Toy problem

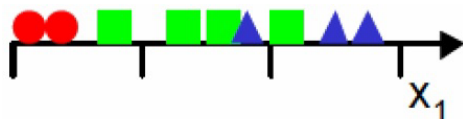
We consider a Pattern Recognition problem with 3 classes. We have 9 available observation represented in 1 dimension.



A simple approach would be to do the following:

- Divide the feature space into uniform bins.
- Compute the class ratio in each bin and use a majority vote to classify the bin.
- When a new example comes, put it in its closest bin.

# The Toy problem



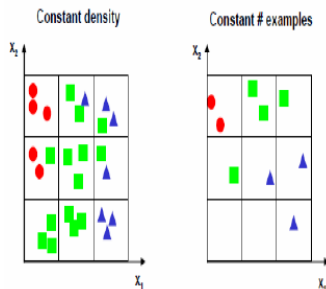
- In this first example with one feature, we observe that when dividing the space into 3 segments we get 3 homogeneous regions each with a similar density of 3 examples per bin.
- We also see that there is too much overlap between the classes, so we decide to add a second feature to try to improve the class separability.

## The Toy problem 2D

- If we add a 2nd dimension we pass from 3 cases in 1D to  $3^2 = 9$  in 2D.
- We have an another problem: do we maintain the density of examples per bin or do we keep the same number of example than in 1D?

# The Toy problem 2D

- If we add a 2nd dimension we pass from 3 cases in 1D to  $3^2 = 9$  in 2D.
- We have an another problem: do we maintain the density of examples per bin or do we keep the same number of example than in 1D?

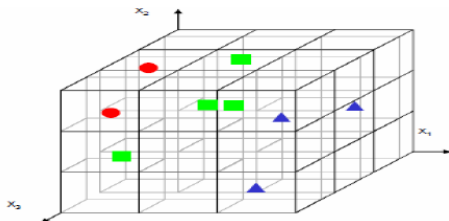


- If we want to maintain the density, we now need 27 examples instead of 9.
- Choosing to maintain the number of examples to 9 will result in a very sparse 2D scatter plot.

# The Toy problem 3D

Adding a 3rd dimension makes the problem worse:

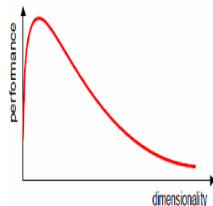
- We move to  $3^3 = 27$  bins.
- Keeping a constant density now requires 81 observations.
- Keeping the same number of observation gives us an almost empty 3D plot.



# The curse of dimensionality

The curse of dimensionality generates several phenomena such as:

- The concentration of observations in given space areas
- The desertification of the data space
- The depopulation of the center of hyper-volumes



In practice, the curse of dimensionality means that, for a given sample size, there is a maximum number of variables beyond which a classifier performance will degrade rather than improve.

The approach used on the toy example is mostly ineffective:

- There are other approaches less affected by the curse of dimensionality, but the problem will still exist and will always re-surface at some point.

# Consequences of the curse of dimensionality

- Exponential growth of the number of examples required to maintain a given sample density: For a density of  $N$  examples/bin in  $D$  dimensions,  $N^D$  examples are required.
- Exponential growth of the complexity of the target function (which estimates the density). To learn well, the target function requires a dense enough learning space.
- For one dimension, we have plenty of different density functions. However, for high dimension, we only have the Gaussian multivariate density. For large values of  $D$ , the density can only be treated in Gaussian simplified forms (due to the inverse covariance matrix in the Gaussian mixture model).



# How to deal with the curse of dimensionality ?

These findings suggest that we need special treatment to manipulate high dimensional data:

- Incorporating prior knowledge to reduce the search space.
- Providing smoother and more generic target functions.
- Reducing dimensionality.

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- Reducing dimensionality.

## Reducing dimensionality

The reduction of dimensionality by the mean of space transformations, projections, or feature selection is usually the preferred solution in combination with the two others.

- Prior knowledge is not always available, and may alone result in over-fitting.
- Smoother target functions alone may result in a global decrease of performances and are cumbersome to design.

# Dimension Reduction

Dimension reduction is based on the hypothesis that high dimensional data are not uniformly distributed:

- There are high density and low density areas.
- Dimension reduction looks for structures that define these high and low density areas to tackle the curse of dimensionality.

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There are many techniques of dimension reduction:

- Linear and non-linear
- Deterministic and probabilistic
- Supervised and unsupervised

# Selection vs Extraction

There are two main methodology for dimension reduction:

- **Feature selection:** Choosing a subset of all the features.
- **Feature extraction:** Creating a small set of new features by combinations of the original ones.

$$\begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_D \end{bmatrix} \xrightarrow{\text{feature selection}} \begin{bmatrix} X_{i_1} \\ X_{i_2} \\ \vdots \\ X_{i_M} \end{bmatrix}$$

$$\begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_D \end{bmatrix} \xrightarrow{\text{feature extraction}} \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_M \end{bmatrix} = f \left( \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_D \end{bmatrix} \right)$$

# Outline

- 1 Introduction
- 2 Feature selection methods**
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# Feature selection

## Definition

Variable selection is a process to choose an optimal subset of relevant variables from a set of variables, according to a performance criterion.

We can ask three basic questions:

- Q1 How to measure the relevance of the variables ?
- Q2 How to obtain the optimal subset ?
- Q3 Which optimality criterion to use ?

# Feature selection

Q1 How to measure the relevance of the variables ?

- We need to find a measure of relevance, or evaluation criterion  $J(X)$ , to quantify the importance of one variable or a combination of variables.



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Q3 Which optimality criterion to use ?

- With the answer to Q2 being an optimization algorithm, we need to define a stopping criterion for this optimization process.

## Choosing a criterion for feature selection: Examples

- For a **Classification problem**, we can test the discriminant quality of the system in the presence presence or absence of a variable.
- For a **Regression problem**, we can test the quality of the prediction with respect to the other variables.

## Feature selection: Branch & Bound based methods

**Branch & Bound** based methods use an optimization strategy that finds the optimal subset of variable based on a minimal bound to reach on the evaluation criterion.

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- 4 When there is no feature left to try removing, the algorithm remembers the best score and backtracks to another branch.
- 5 The algorithm stops when all branches with valid subsets have been tested.

## Monotonic VS non-monotonic feature selection criteria

Branch & Bound methods can only work if the selection criterion  $J(X)$  is monotonic.

### Monotonic criterion: Definition

Let us consider two subsets of features  $A_1$  and  $A_2$ . Then,  $J(\cdot)$  is monotonic if and only if  $A_1 \subset A_2 \implies J(A_1) \leq J(A_2)$ .

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**Problem:** Most effective evaluation criteria are not monotonic ...

The use of sub-optimal methods is then required:

- Sequential Forward Selection (SFS)
- Sequential Backward Selection (SBS)
- Bidirectional Selection (BS)

# Sequential Forward Selection

Let  $X = \{X_1, \dots, X_D\}$  be a set of variables. The SFS procedure is the following:

- Initially set the selected set of variables  $A_0$  as empty.
- At each step  $k$ , select the variable  $X_i$  that maximizes the following criterion of evaluation  $J(A_k)$ :

$$J(A_k) = \max_{X_i \in (X \setminus A_{k-1})} J(A_{k-1} \cup X_i)$$

This will result in a list of variables ordered by their importance. The procedure can be stopped at any step when a given criterion (e.g. acceptable loss of information) has reached an acceptable value.

# Sequential Backward Selection

Let  $X = \{X_1, \dots, X_D\}$  be a set of variables. The SBS procedure is the following:

- Initially start with a set  $A_D = X$  containing all the variables.
- At each step for  $k \in [D - 1 \dots 1]$ , remove the variable  $X_i$  of the least importance according to:

$$J(A_k) = \max_{X_i \in A_{k+1}} J(A_{k+1} \setminus X_i)$$

This will also result in a list of variables ordered by their importance, with the most important being at the end of the list. The procedure can also be stopped as soon as the remaining set is below an acceptable lower bound of accuracy on a given criterion.

## Bidirectional Selection

The Bidirectional Selection procedure performs the search in both Forward and Backward direction in a competitive manner:

The procedure stops when one of the following case occurs:

- One of the two direction has found the best subset of variables before reaching the middle of the search space.
- The two branches are reaching the middle.

This method reduces the search time as the search is performed in both directions and stops when there is a solution regardless of the direction.

### Remark

The sets of best selected variables found respectively by SFS and SBS are not equal and rarely identical because of their different principles of selection.

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# Feature Extraction: Principle

Feature extraction consists in building new features from the original ones with one or several of the following goals:

- Having a lower number of features while keeping a maximum of information
- Having better features with which the data are easier to process
- Having feature with which the data are easier to visualize

$$\begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_D \end{bmatrix} \xrightarrow{\text{feature extraction}} \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_M \end{bmatrix} = f \left( \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_D \end{bmatrix} \right)$$

# Types of feature extraction methods

## Linear Methods

- Principal components Analysis (PCA)
- Linear Discriminant Analysis (LDA)
- Multi-Dimensional Scaling (MDS)
- ...

## Non-linear methods

- Isometric feature mapping (Isomap)
- Locally Linear Embedding (LLE)
- Kernel PCA
- Spectral clustering
- Supervised methods (S-Isomap)
- ...

## Reducing the dimensionality: goals

*The Principal Component Analysis (PCA) is a method of data analysis and dimensionality reduction that seeks the directions of space that best represent the correlations between  $D$  random variables.*

### Goals

- 1 Obtaining an approximation of a scatter of  $K$  objects in a subspace of low dimension (2 or 3).
- 2 Summarizing a data set represented by a matrix  $X$  of  $N$  rows and  $D$  columns.
- 3 Getting a simple and reliable visualization of the information contained in the data.

## Reducing the dimensionality: Principle of PCA

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# Reducing the dimensionality: Principle of PCA

*The Principal Component Analysis (PCA) is a method of data analysis and dimensionality reduction that seeks the directions of space that best represent the correlations between  $D$  random variables.*

## Principle

- 1 Compute the covariances or correlations between variables.
- 2 Use this indexes to create new variables:
  - The original variables are replaced with the new variables.
  - Each new variable is a linear combination of the original variables.
  - These new variables must be as independent (uncorrelated) from each other as possible.
- 3 Select among the new variables the ones that best represent the distribution of the data and eliminate the others.

# PCA : Principle

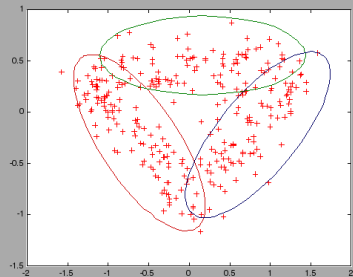
## Breiman Waveform

```

-1.23,-1.36,-1.75,-0.28,0.60,2.72,0.85,0.21,-0.20,0.89,1.08,4.20,2.88,7.75,4.39,3.15,5.32,3.32,1.20,0.24,-0.56,2
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-0.51,-0.48,0.35,-1.67,0.26,2.45,-0.09,2.03,0.79,1.42,1.13,2.52,2.66,4.50,4.28,4.66,3.30,0.38,0.75,1.78,0.37,0
1.16,-1.19,-2.26,0.63,0.32,1.33,2.13,2.58,1.03,2.91,4.04,4.55,5.65,2.74,3.32,2.67,2.01,4.12,-0.81,0.97,-0.98,2
-0.09,2.30,-0.40,0.36,0.11,-1.20,1.47,2.23,1.50,2.14,6.48,5.45,2.22,2.79,2.61,1.87,0.46,1.98,1.64,1.32,0.73,2
-1.43,-0.46,-0.32,1.45,-0.50,1.35,1.39,0.81,0.03,1.35,2.55,2.42,3.07,5.46,6.29,6.50,4.60,3.77,1.62,1.01,-1.86,0

```

PCA



**Figure:** From 21 variables to 2 variables using PCA. Note that the 3 clusters are still visible.

# PCA and Normalizing the data: Centering and reducing

Prior to a Principal Component Analysis, centering the variables around their means and scaling them may be necessary.

## Centered variables

$$M = \begin{pmatrix} x_{1,1} - \mu_1 & \cdots & x_{1,D} - \mu_D \\ \vdots & \ddots & \vdots \\ x_{N,1} - \mu_1 & \cdots & x_{N,D} - \mu_D \end{pmatrix}$$

## Centered Reduced variables

$$\tilde{M} = \begin{pmatrix} \frac{x_{1,1} - \mu_1}{\sigma_1} & \cdots & \frac{x_{1,D} - \mu_D}{\sigma_D} \\ \vdots & \ddots & \vdots \\ \frac{x_{N,1} - \mu_1}{\sigma_1} & \cdots & \frac{x_{N,D} - \mu_D}{\sigma_D} \end{pmatrix}$$

# PCA and the Variance-Covariance Matrix

Once the data have been normalized, computing the variance-covariance matrix is the next step in order to assess the potential relationships between the different variables.

## Variance-Covariance

$$C = \begin{pmatrix} \text{VAR}(X_1) & \cdots & \text{COV}(X_1, X_D) \\ \vdots & \ddots & \vdots \\ \text{COV}(X_D, X_1) & \cdots & \text{VAR}(X_D) \end{pmatrix}$$



## Calculation of new PCA variables

Now that we know the covariance relationships between all variables, we seek to create new variables using linear combinations of the old ones:

- A first new variable represented by a single axis  $u_1$  so that the projection of  $u_1$  has a maximum variance.
- Then we seek for a second axis  $u_2$  independent of  $u_1$  (i.e. orthogonal to  $u_1$ ) that best explains the remaining variance.
- And so on.

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- And so on.

Note that for visualization purposes, 2 or max 3 axes are usually enough.

# PCA : Example 1

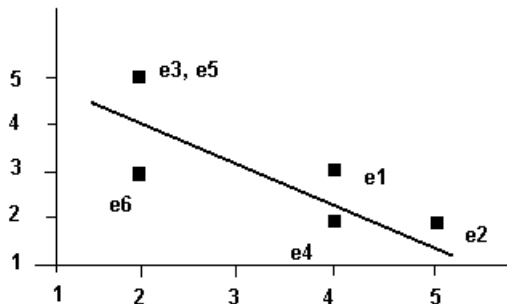


Figure: A possible projection on a new single axis

## PCA : Example 2

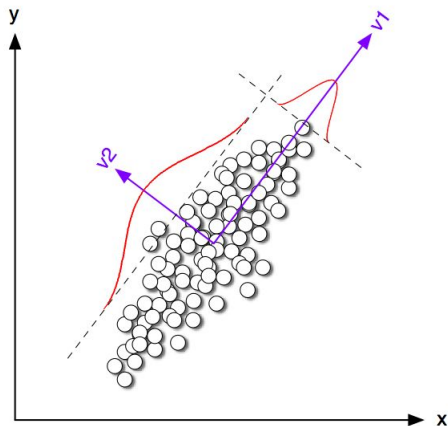


Figure: Changing the axis for more convenient variables

# PCA : Example 3

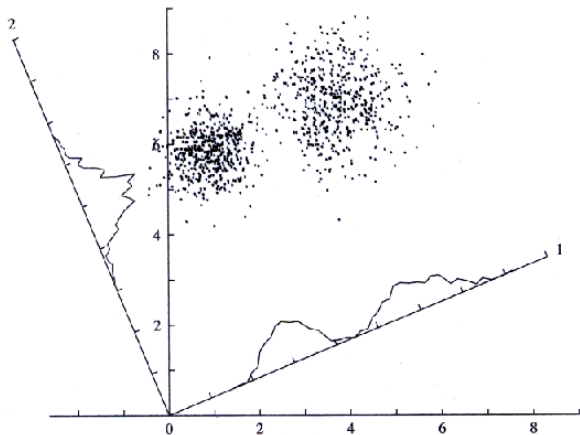


Figure: A possible projection on two new axis

## PCA : Calculating the new variables (1/6)

Let us denote  $M$  the centered version of the data set  $X$  of  $n$  rows and  $d$  columns,  $u_1$  the first loading vector, and  $\pi_{u_1}(M) = M \cdot u_1$  the projection of the data set on this component.

- We seek  $u_1$  of norm 1 so that the projection of the data on  $u_1$  has a maximum variance.

### Computing $u_1$

$$u_1 = \operatorname{argmax}_{\|u\|=1} \left( \sum_{i=1}^p (\pi_u(M_i))^2 \right)$$

$$u_1 = \operatorname{argmax}_{\|u\|=1} (\|M \cdot u\|^2) = \operatorname{argmax}_{\|u\|=1} (u^T \cdot M^T M \cdot u)$$

## PCA : Calculating the new variables (2/6)

- We seek  $u_1$  of norm 1 so that the projection of the data on  $u_1$  has a maximum variance.

### Computing $u_1$

Let us note  $V_\pi$  the variance of  $\pi_u(M)$ :

$$V_\pi = \frac{1}{N-1} \pi_u(M)^T \cdot \pi_u(M) = u^T \cdot \underbrace{\frac{M^T M}{N-1}}_C \cdot u = u^T \cdot C \cdot u$$

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- With  $C$  the variance-covariance matrix of the original dataset  $X$ .



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- With  $C$  the variance-covariance matrix of the original dataset  $X$ .
- Note that it only works because all variables  $M_i$  are centered !

## PCA : Calculating the new variables (3/6)

### Computing $u_1$

From  $V_\pi = u^T \cdot C \cdot u$ , maximizing  $V_\pi$  is equivalent to solve:

$$C \cdot u = V_\pi \cdot u$$

By definition, the solution of this equation is the set of couples :  
eigenvectors / eigenvalues of  $C$ .

- The largest eigenvalue  $\lambda_1$  is the variance  $V_\pi$ , the maximum reachable.
- The associated eigenvector is the projection axis  $u_1$  along which  $V_\pi$  is maximum.

## PCA : Calculating the new variables (4/6)

The above reasoning has allowed us to conclude that the vector which explains the more inertia (i.e. the variance) of the data points is the first eigenvector. Similarly, the second vector which explains most of the remaining inertia is the second eigenvector, etc.

- We also saw that the variance of the data projected onto the  $n^{\text{th}}$  eigenvector (also called - variance explained by this axis) is  $\lambda_n$ .

### Remark

In Matrix form, we have:  $C \propto U\Lambda U^T$  where  $\Lambda$  is a diagonal matrix containing all single values.

# PCA : Calculating the new variables (5/6)

## Computing $u_k$

To find the  $k^{th}$  component, the data are updated:

$$\tilde{X}_k = X - \sum_{s=1}^{k-1} X \cdot u_s \cdot u_s^T$$

The process that we have just presented is repeated by finding the new maximal eigenvectors of the variance-covariance matrix of the new data.

# PCA : Calculating the new variables (5/6)

## Computing $u_k$

To find the  $k^{th}$  component, the data are updated:

$$\tilde{X}_k = X - \sum_{s=1}^{k-1} X \cdot u_s \cdot u_s^T$$

The process that we have just presented is repeated by finding the new maximal eigenvectors of the variance-covariance matrix of the new data.

It turns out that this process gives the remaining eigenvectors of the original variance-covariance matrix.

- Therefore, in practice the  $k^{th}$  component is picked by choosing the  $k^{th}$  largest eigenvalue and the associated eigenvector.

# PCA : Calculating the new variables (6/6)

## Algorithm

- 1 Choose  $p$  the number of dimensions that you want to keep.
- 2 Select the eigenvectors  $(u_1, \dots, u_p)$  associated with the  $p$  largest eigenvalues.
- 3 Project the data on the new axes in order to obtain a description of these data according to the new variables (called principal components):  $\pi_u(M) = M \cdot u$ .
- 4 If the number of dimensions is  $\leq 3$ , it is possible to represent the data in the new space.

# PCA : Calculating the new variables

## Another possible algorithm

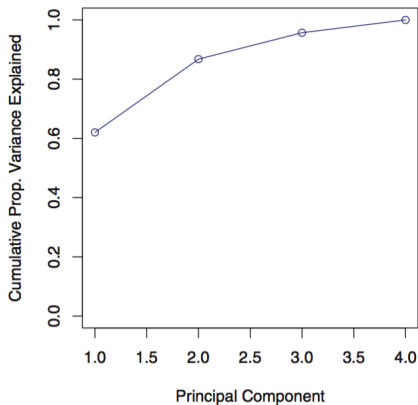
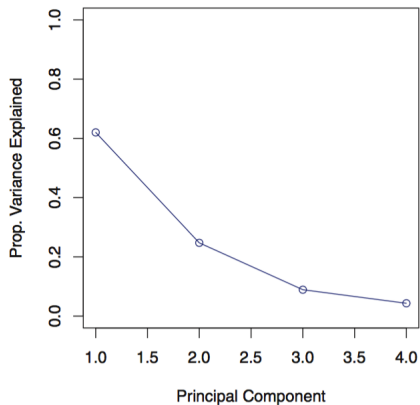
- 1 Choose  $P$  the proportion of information (also called inertia) that we want to keep.
- 2 Select  $y$  eigenvectors so that:

$$y = \underset{y}{\operatorname{argmin}} \frac{\sum_{i=1}^y \lambda_i}{\sum \lambda} \geq P$$

- 3 Project the data on the new axes.
- 4 If the number of dimensions is  $\leq 3$ , it is possible to represent the data in the new space.

# PCA : choosing the number of components

We typically decide on the number of principal components required by examining a scree plot. Look for a point at which the proportion of variance explained by each subsequent principal component drops off, this is often referred to as an *elbow* in the scree plot.





## Reminders

### Reminder: eigenvalues

The eigenvalues of a matrix  $X$  are determined by the vector  $\lambda$  so that:

$$|X - \lambda I| = 0$$

Where  $|\cdot|$  is the determinant operator.

### Reminder: eigenvectors

The eigenvector  $v_i$  linked to a eigenvalue  $\lambda_i$  solves the following equation:

$$X \cdot v_i = \lambda_i \cdot v_i$$

# Computing the correlations

We know that the new variables represent linear combinations of the old ones. It is therefore interesting to analyze the correlation between the old and new variables to interpret the results.

## Correlations between an old variable and a new variable

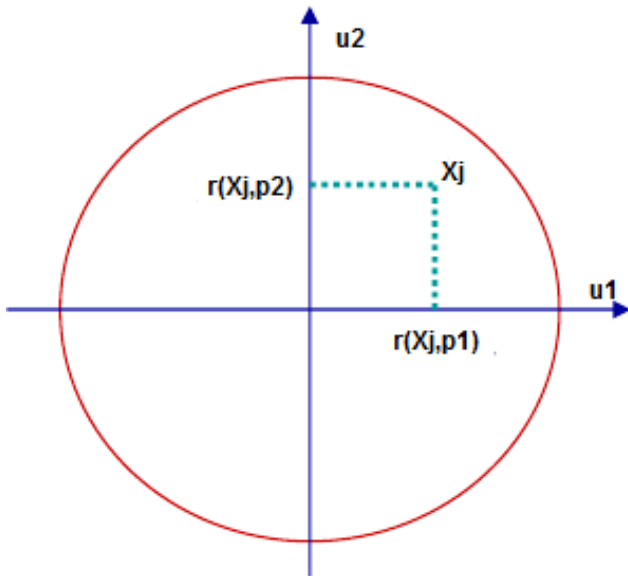
$$r(M_i, \pi_j) = \frac{1}{N} \frac{\sum M_i \cdot \pi_j}{\sigma_i \sqrt{\lambda_j}}$$

This expression follows directly the original formula for the correlation coefficient, recalling that  $\lambda_j$  is the variance of the projection of the data on the new  $u_j$  axis.

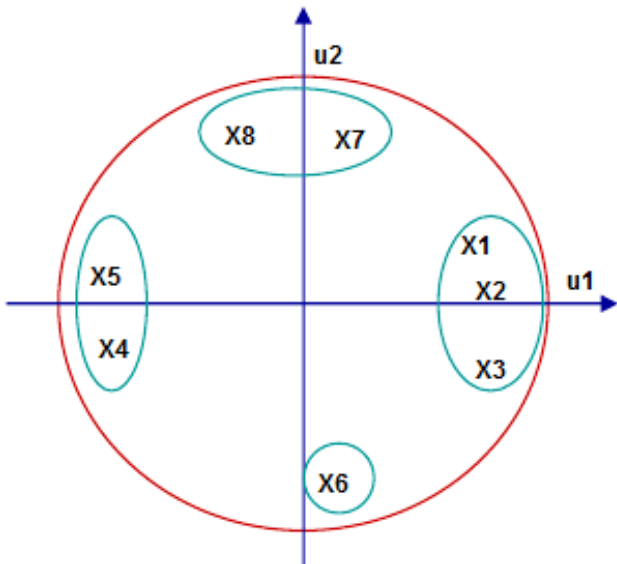
## Circle of correlations (1/3)

- Now that we know the correlation between the old and new variables, we can simply visualize a **circle of correlations**.
- This allows to both characterize the new variables (which makes it possible to visually interpret the data) and to visualize the correlation between the old variables.

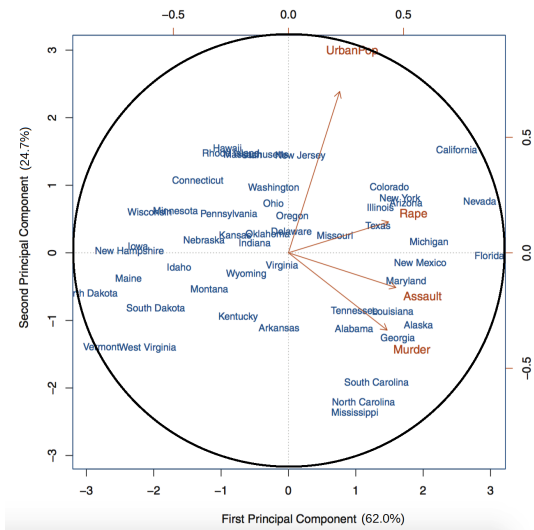
## Circle of correlations (2/3)



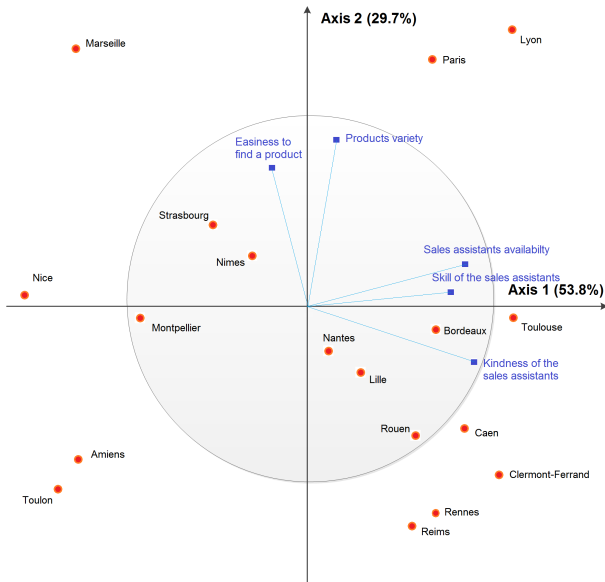
# Circle of correlations (3/3)



# Circle of correlations: Example



# Circle of correlations: Example



# Limits of PCA

## The problem with PCA

- Using PCA for large data sets with many attributes ?
  - Examples: genetic data, text data
  - The covariance matrix is of size  $d \times d$ . If there are too many attributes, computing the eigenvalues is too computationally expensive because the matrix is too big.
- Solution: Singular Value Decomposition (SVD)
  - Powerful algorithms exist in Python, R, matlab and SAS to compute it.
- When to use SVD ?
  - More attributes than data:  $N < D$
  - When the centered data matrix  $M$  contains mostly 0 (sparse data).



# Principle

## SVD

Given a centered data matrix  $M$ , the goal of the SVD is to find the matrices  $U$ ,  $S$  and  $V$  to achieve the following decomposition:

$$M = USV^T$$

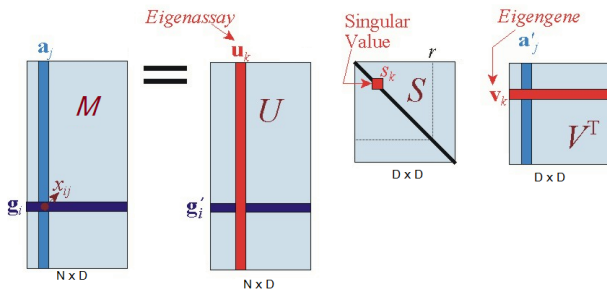
- $M$  The data centered data matrix of size  $N \times D$
- $U$  The matrix containing the left singular vectors (eigenassay), of size  $N \times D$ .
- $S$  The diagonal matrix containing the singular values, of size  $D \times D$
- $V^T$  The matrix containing the right singular vectors (eigengenes), of size  $D \times D$

# Principle

## SVD

Given a centered data matrix  $M$ , the goal of the SVD is to find the matrices  $U$ ,  $S$  and  $V$  to achieve the following decomposition:

$$M = USV^T$$



## Relation to PCA

Let  $C$  be the variance-covariance matrix of  $M$ . Then:

$$C = \frac{M^T M}{N - 1}$$

With the SVD, we have  $M = USV^T$ , therefore:

$$C = \frac{VSU^TUSV^T}{N - 1} = V \frac{S^2}{N - 1} V^T$$

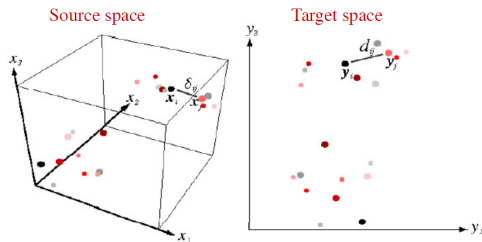
Thus:

- The eigenvalues can be computed from the singular values  $\lambda_i = \frac{s_i^2}{N-1}$
- $V$  stores the eigenvectors of  $M^T M$ .

# Multi-dimensional scaling

Multi-dimensional scaling (MDS) originally proposed by Borg and Groenen in 1997:

- MDS encompasses a collection of reduction techniques that maps the distances between observations in a high dimensional space into a lower dimensional one.
- It aims at finding a configuration of the points in the low dimensional space so that the inter-point distances remain mostly proportional to the one in higher dimension.



# Multi-dimensional scaling

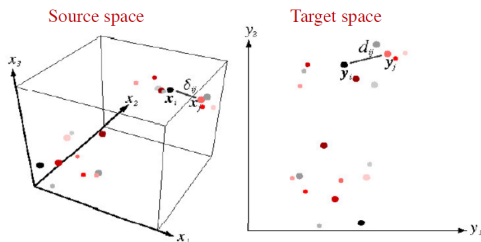
Besides dimension reduction, MDS is well suited for applications or algorithms based on the distances between the data, rather than the data themselves:

- Re-building the map of a country based on the distance between the cities.
- Building a 2D map from 3D coordinates (e.g. star constellation map).
- etc.

## Remarks

- With  $\frac{N(N-1)}{2}$  distances, it is always possible to generate the position of  $N$  points in a  $N$  dimension space.
- MDS computes an approximation for a lower dimensional space.

# Multi-dimensional scaling: Problem formulation



## We have

- The points  $x_1, \dots, x_N$  in  $D$  dimensions
- Any distance  $\delta_{ij}$  between points  $x_i$  and  $x_j$

## We want to find

- The points  $y_1, \dots, y_N$  in 2 or 3 dimensions
- The distance  $d_{ij}$  between any  $y_i$  and  $y_j$  so that it is close to  $\delta_{ij}$

# Multi-dimensional scaling: Cost function

- We must search  $d_{ij}$  so that it minimizes an objective function.
- We can define such function in a general manner:

$$Cost = \sum_{i < j} (d_{ij} - \delta_{ij})^2$$

$$\delta_{ij} = \|x_i - x_j\|^2$$

$$d_{ij} = \|y_i - y_j\|^2$$

## Multi-dimensional scaling: Stress functions

Given that  $d_{ij}$  is a function of  $y_i$  and  $y_j$  (the  $\delta_{ij}$  are constant), thereafter are a few possible objective functions:

$$J_{aa} = \frac{\sum_{i<j} (d_{ij} - \delta_{ij})^2}{\sum_{i<j} \delta_{ij}^2} \quad \text{penalizes large absolute errors}$$

$$J_{rr} = \sum_{i<j} \left( \frac{d_{ij} - \delta_{ij}}{\delta_{ij}} \right)^2 \quad \text{penalizes large relative errors}$$

$$J_{ar} = \frac{1}{\sum_{i<j} \delta_{ij}} \sum_{i<j} \frac{(d_{ij} - \delta_{ij})^2}{\delta_{ij}} \quad \text{A compromise between the two}$$

The last one,  $J_{ar}$ , is also referred as **Sammon Criterion**.



# Multi-dimensional scaling: Algorithm

- Choose an objective function  $J$  and a step parameter  $0 < \eta < 1$ .
- Compute the distances  $\delta_{ij}$  if they are not provided.
- Initialize the points  $y_1, \dots, y_N$  randomly and compute the corresponding  $d_{ij}$ .
- Repeat until convergence:

$$\forall i \quad y_i \leftarrow y_i - \eta \nabla J(y_i)$$

# Multi-dimensional scaling: Update Rule

$$\nabla J_{aa}(y_k) = \frac{2}{\sum_{i < j} \delta_{ij}^2} \sum_{j \neq k} (d_{kj} - \delta_{kj}) \frac{y_k - y_j}{d_{kj}}$$

$$\nabla J_{rr}(y_k) = 2 \sum_{j \neq k} \frac{d_{kj} - \delta_{kj}}{\delta_{kj}^2} \frac{y_k - y_j}{d_{kj}}$$

$$\nabla J_{ar}(y_k) = \frac{2}{\sum_{i < j} \delta_{ij}} \sum_{j \neq k} \frac{d_{kj} - \delta_{kj}}{\delta_{kj}} \frac{y_k - y_j}{d_{kj}}$$

# Multi-dimensional scaling: Example 1

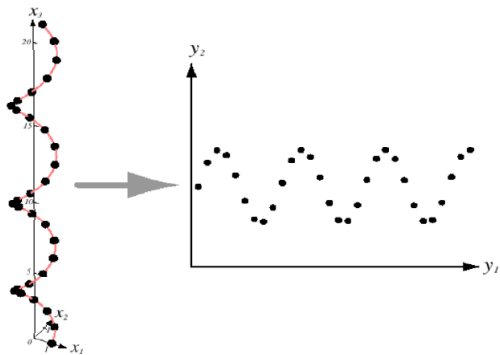


Figure: From 3D to 2D using MDS

## Multi-dimensional scaling: Example 2

- The dataset "Eurodist" represents the distance in kilometers between 21 European cities.
- The source data set is a square matrix containing the distances between the cities:

	Athens	Barcelona	Brussels	Calais	Cherbourg	Cologne	Copenhagen	Geneva	Gibraltar	Hamburg
Barcelona	3313									
Brussels	2963	1318								
Calais	3175	1326	204							
Cherbourg	3339	1294	583	460						
Cologne	2762	1498	206	409	785					
Copenhagen	3276	2218	966	1136	1545	760				
Geneva	2610	803	677	747	853	1662	1418			
Gibraltar	4485	1172	2256	2224	2047	2436	3196	1975		
Hamburg	2977	2018	597	714	1115	460	460	1118	2897	

## Multi-dimensional scaling: Example 2

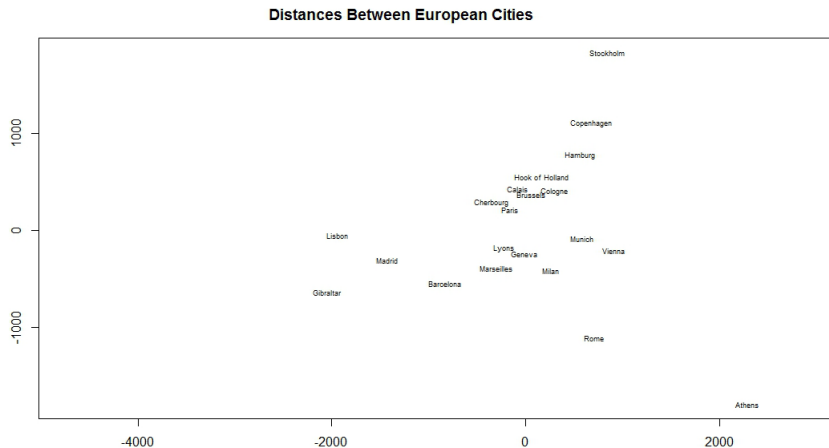


Figure: Reconstructed map of Europe using MDS

# Multi-dimensional scaling: Conclusions

The different MDS algorithms differ in the following points:

- The distance used in the source space.
- The Stress (objective) functions: Using a different stress function will lead to a different result.
- The optimization procedure: Linear MDS can be solved analytically but cannot model complex (non-linear) low dimensional manifolds well. However, non-linear MDS requires a more complex and iterative algorithm.

# Outline

- 1 Introduction
- 2 Feature selection methods
- 3 Linear Feature extraction methods
- 4 Bibliography**

# Bibliography

- Christopher M. Bishop, Pattern Recognition and Machine Learning (2006)
- Tom M. Mitchell, Machine Learning (1997)