Cluster analysis

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Introduction

Cluster analysis foundations rely on
one of the most fundamental, simple
and very often unnoticed ways (or methods)
of understanding and learning,
which is grouping “objects” into “similar” groups.

Introduction

What is a cluster?

No general accepted definition!!!

A cluster is ...

D1: ... comprised of a number of *similar* objects collected and grouped together

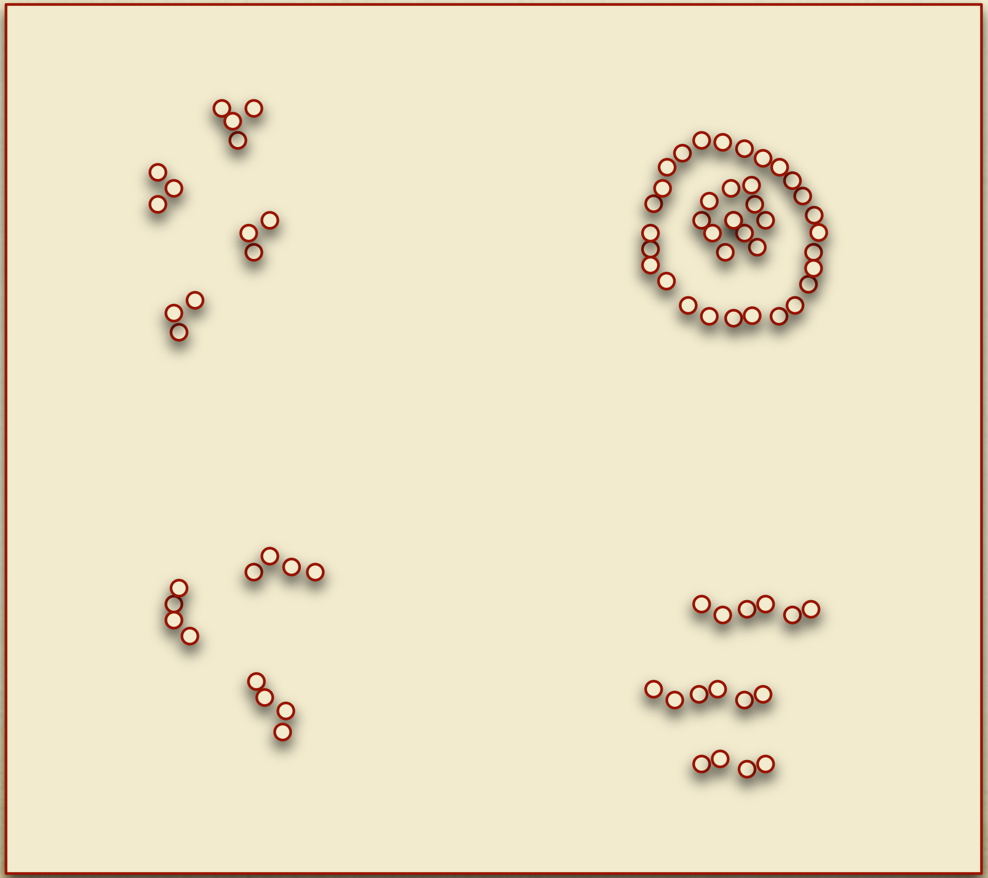
D2: ... a set of entities which are *alike*, and entities from different clusters are not *alike*

D3: ... an aggregation of points in the test space such that the *distance* between any two points in the cluster is less that the distance between any point in the cluster and any point not in it.

D4: ... a connected region of a multidimensional space containing a relative *high density* of points, separated from other such regions by regions containing a relatively low density of points.

Introduction

It is hard to give a general accepted definition of a cluster because objects can be grouped with different purposes in mind.



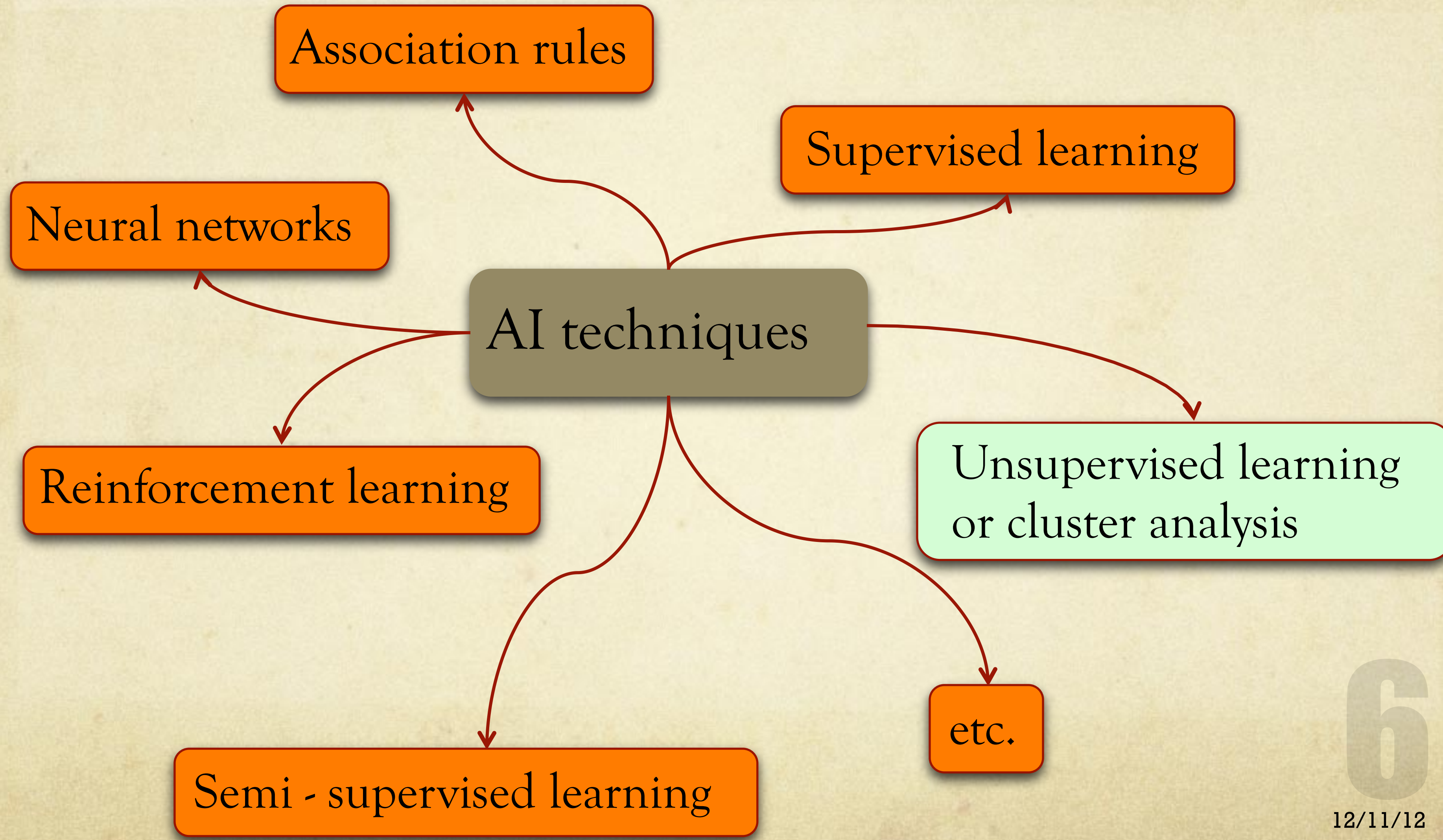
Humans are excellent cluster seekers

...only in two or three dimensions.

Overview

- What is cluster analysis?
- Some definitions and notations
- How it works?
- Cluster Analysis Diagram
    - Objectives of cluster analysis
    - Research design issues
    - Assumptions in cluster analysis
    - Clustering methods
    - Interpreting the clusters
    - Validation
- Applications

What is cluster analysis?



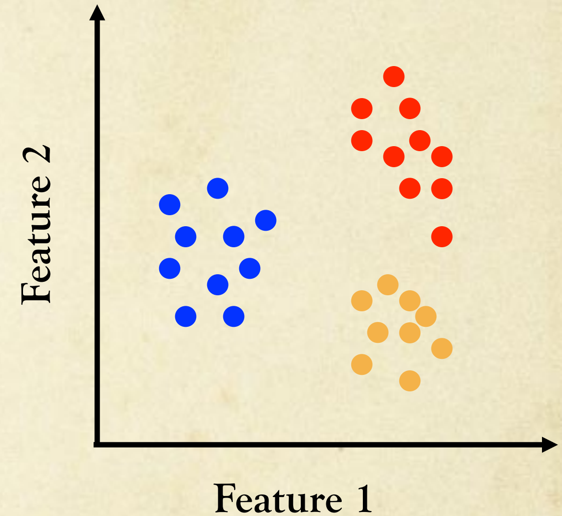
What is cluster analysis?

Cluster analysis is a multivariate data mining technique whose goal is to groups objects based on a set of user selected characteristics

Clusters should exhibit high internal homogeneity and high external heterogeneity

What this means?

When plotted geometrically, objects within clusters should be very close together and clusters will be far apart.



Cluster analysis also referred to as

Exploratory data analysis

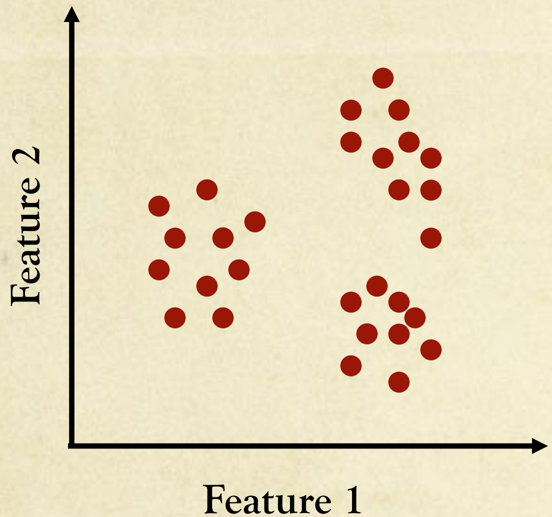
Q analysis

Typology construction

Classification analysis

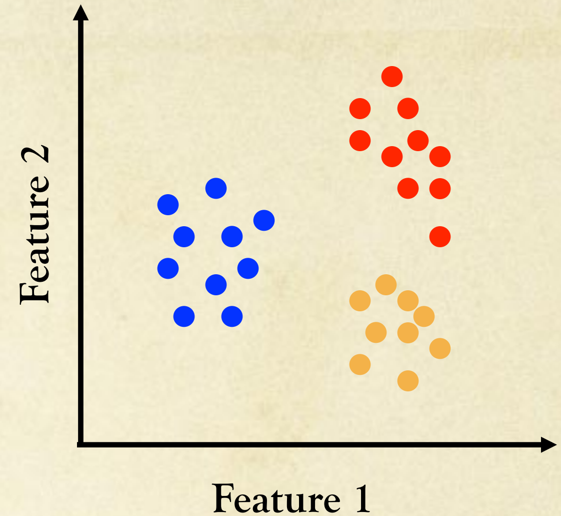
Numerical taxonomy

What is cluster analysis?

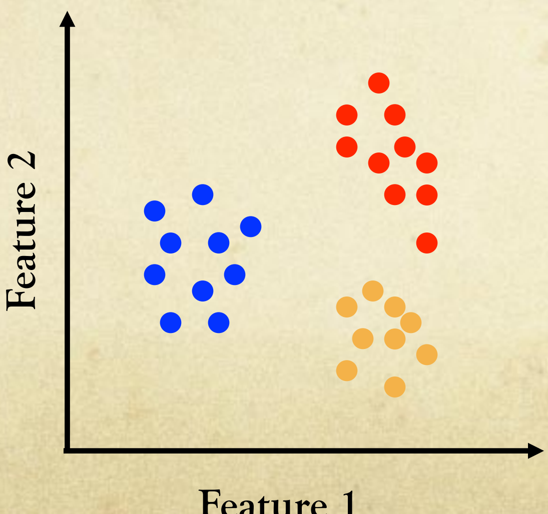


What is?

Clustering or
Unsupervised learning

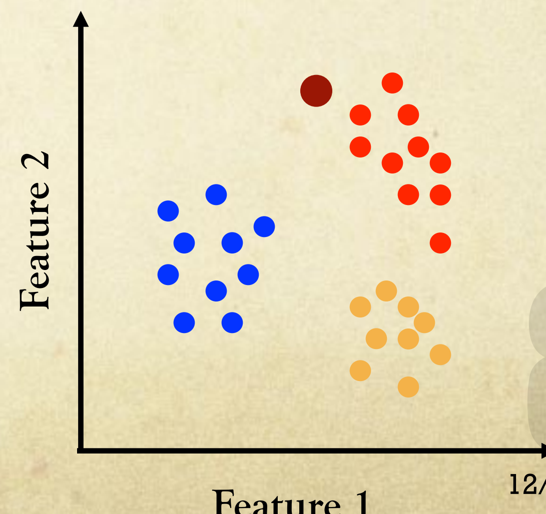


Clustering ≈ natural grouping of data

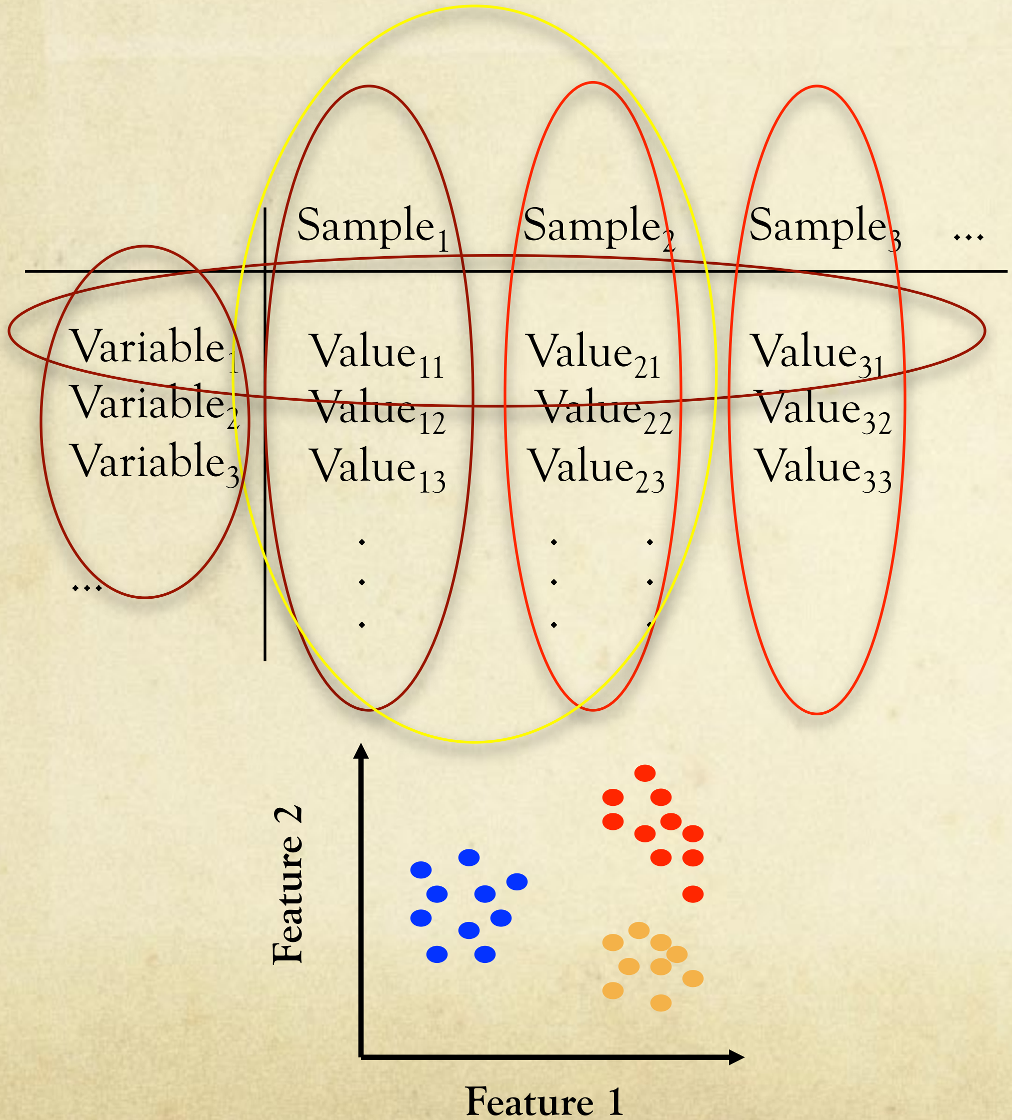


What is not?

Supervised learning



Definitions & notations



- Objects or elementary data
- Features or cluster variate
- Data dimension
- Similarity measure
- Cluster
- Cluster seed
- Cluster centroid
- Cluster solution
- Outlier

Definitions & notations

Dimensions

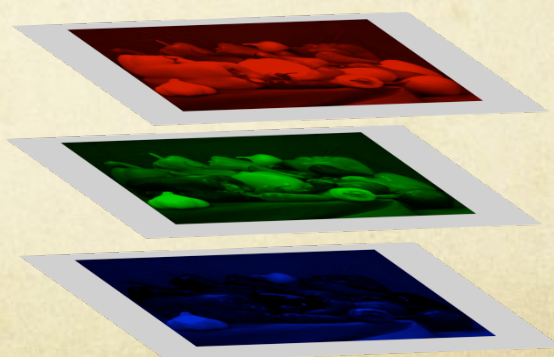
	Sample_1	Sample_2	Sample_3	...
Variable_1	Value_{11}	Value_{21}	Value_{31}	
Variable_2	Value_{12}	Value_{22}	Value_{32}	
Variable_3	Value_{13}	Value_{23}	Value_{33}	
...	⋮	⋮ ⋮		

Number of variables per sample
1 - Univariate data
2 - Bivariate data
3 - Trivariate data
>3 Multi&HyperVariate data

Remark: Quantitative variables (can do math on them)

An example

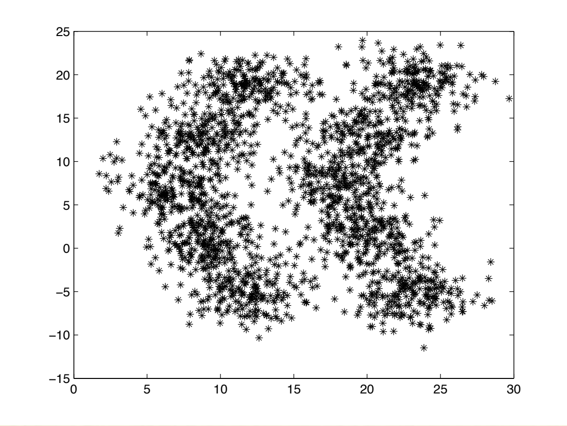
RGB images are trivariate data



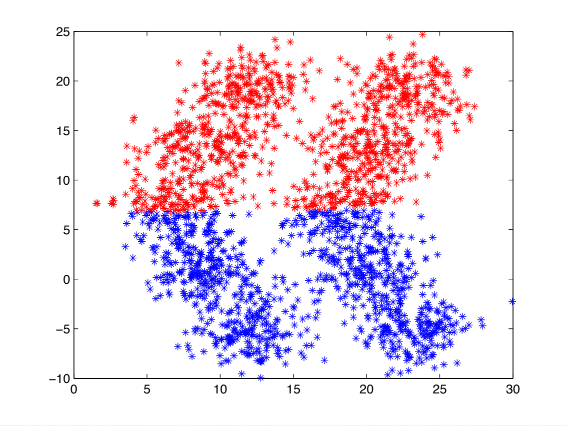
How does it work?

What does *natural grouping* means?

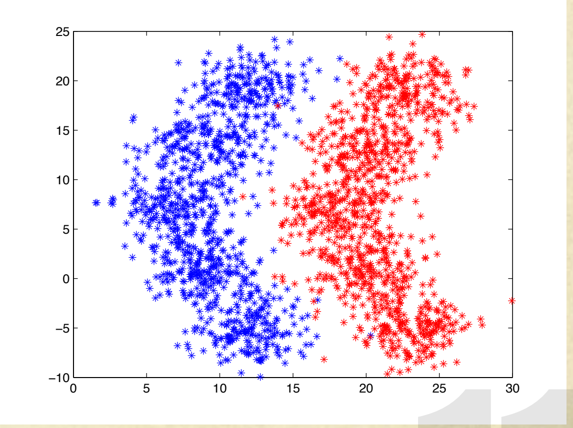
Example



For some clustering algorithms, natural grouping means this…



Actually, natural grouping means this…



How does it work?

Living things

Kingdoms

Phyla (Divisions)

Classes

Orders

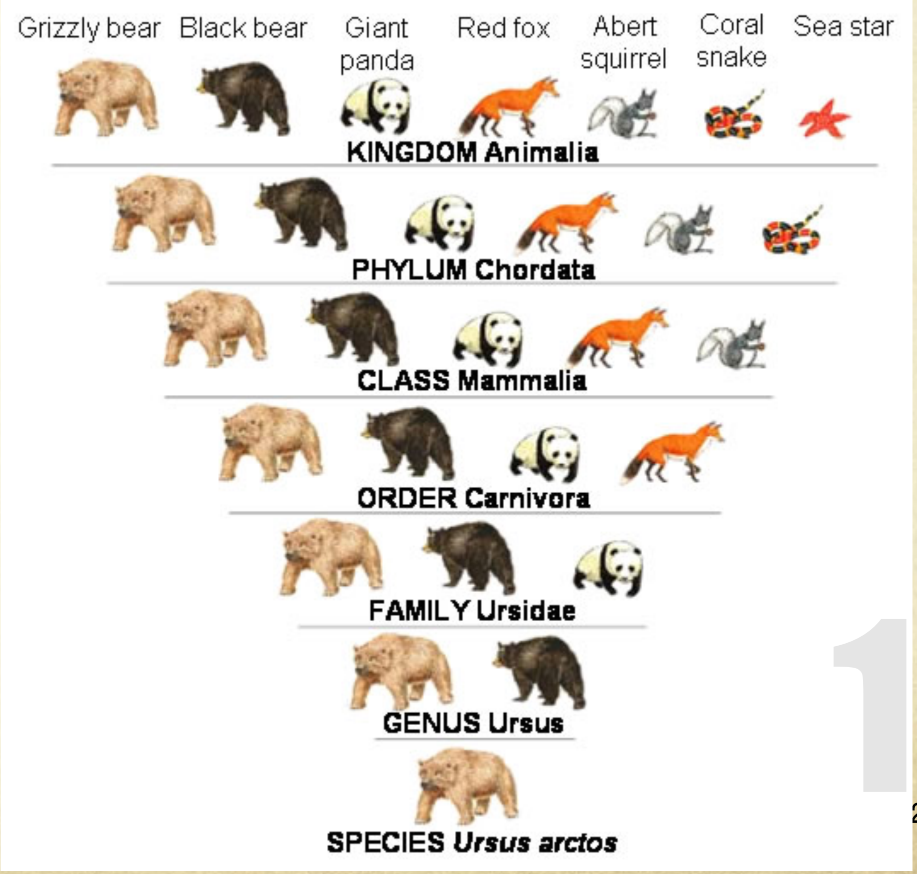
Families

Genera

Species

Samples of living entities

Animalia | Plantae | Protista | Fungi



How does it work?

A simple example:

Suppose that a biologist wants to determine the subspecies in a population of birds belonging the same specie

A small sample of 8 birds is selected as a pilot test

For each of the 8 birds, two characteristics of their beaks are measured: V1 - length and V2 - width.

Clustering variables	Objects							
	S1	S2	S3	S4	S5	S6	S7	S8
V1	3.1	3.3	3.2	3.8	3.65	3.7	3.75	3.78
V2	1.1	1.2	1.05	1.1	1.2	1.05	1.6	1.62

How does it works?

A simple example:

Clustering variables	Objects							
	S1	S2	S3	S4	S5	S6	S7	S8
V1	3.1	3.3	3.2	3.8	3.65	3.7	3.75	3.78
V2	1.1	1.2	1.05	1.1	1.2	1.05	1.6	1.62

Objective

Identify structures (classes) in the data by grouping the most similar objects into groups

Three questions to be answered:

Q1: how does he measure the similarity between individuals?

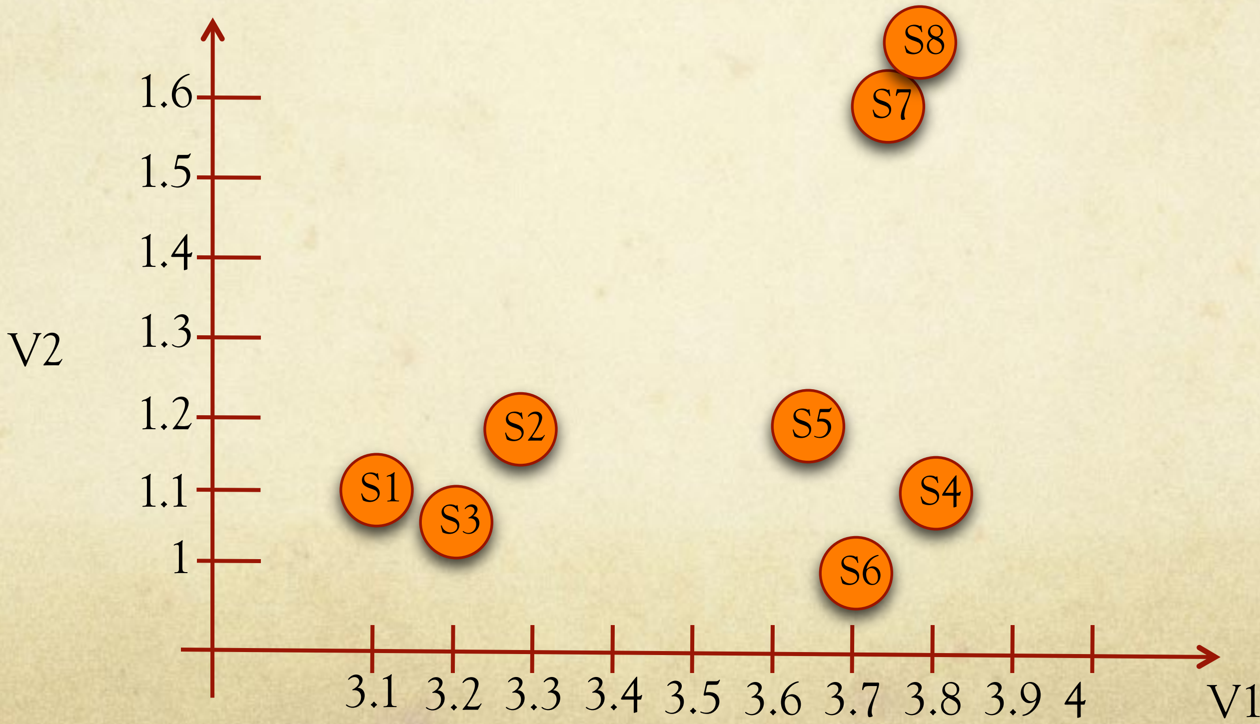
Q2: how clusters should be formed?

Q3: how many clusters?

How does it work?

Q1: how does he measure the similarity between objects?

Clustering variables	Subjects							
	S1	S2	S3	S4	S5	S6	S7	S8
V1	3.1	3.3	3.2	3.8	3.65	3.7	3.75	3.78
V2	1.1	1.2	1.05	1.1	1.2	1.05	1.6	1.62



How does it work?

Q1: how does he measure the similarity between objects?

A1: build similarity matrix between all pairs of observations

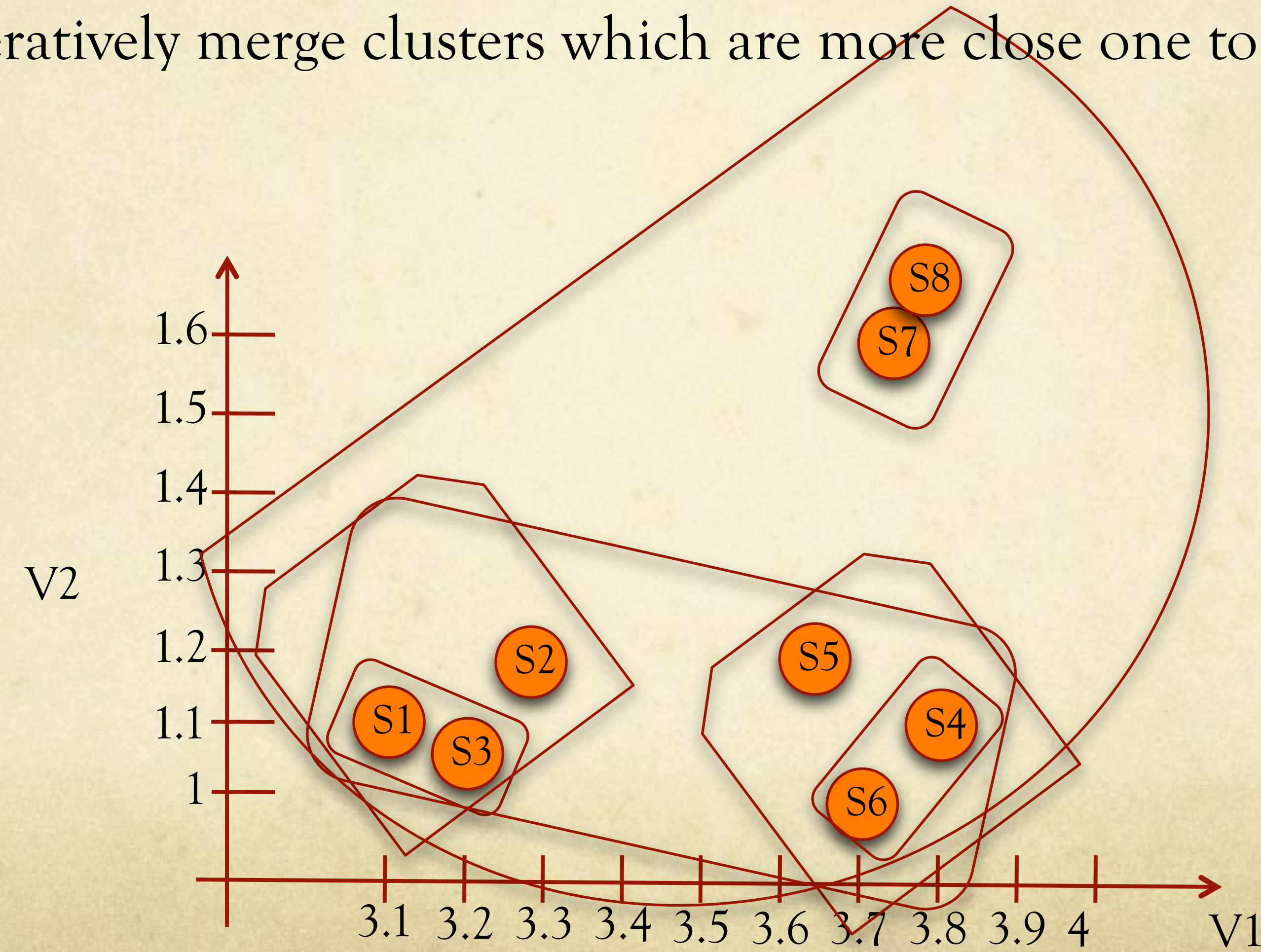
Observations	Observations							
	S1	S2	S3	S4	S5	S6	S7	S8
S1	--------	--------	--------	--------	--------	--------	--------	--------
S2	0.22	--------	--------	--------	--------	--------	--------	--------
S3			--------	--------	--------	--------	--------	--------
S4				--------	--------	--------	--------	--------
S5					--------	--------	--------	--------
S6						--------	--------	--------

How does it work?

Q2: how does he form the clusters?

A21: group observations which are most similar into clusters

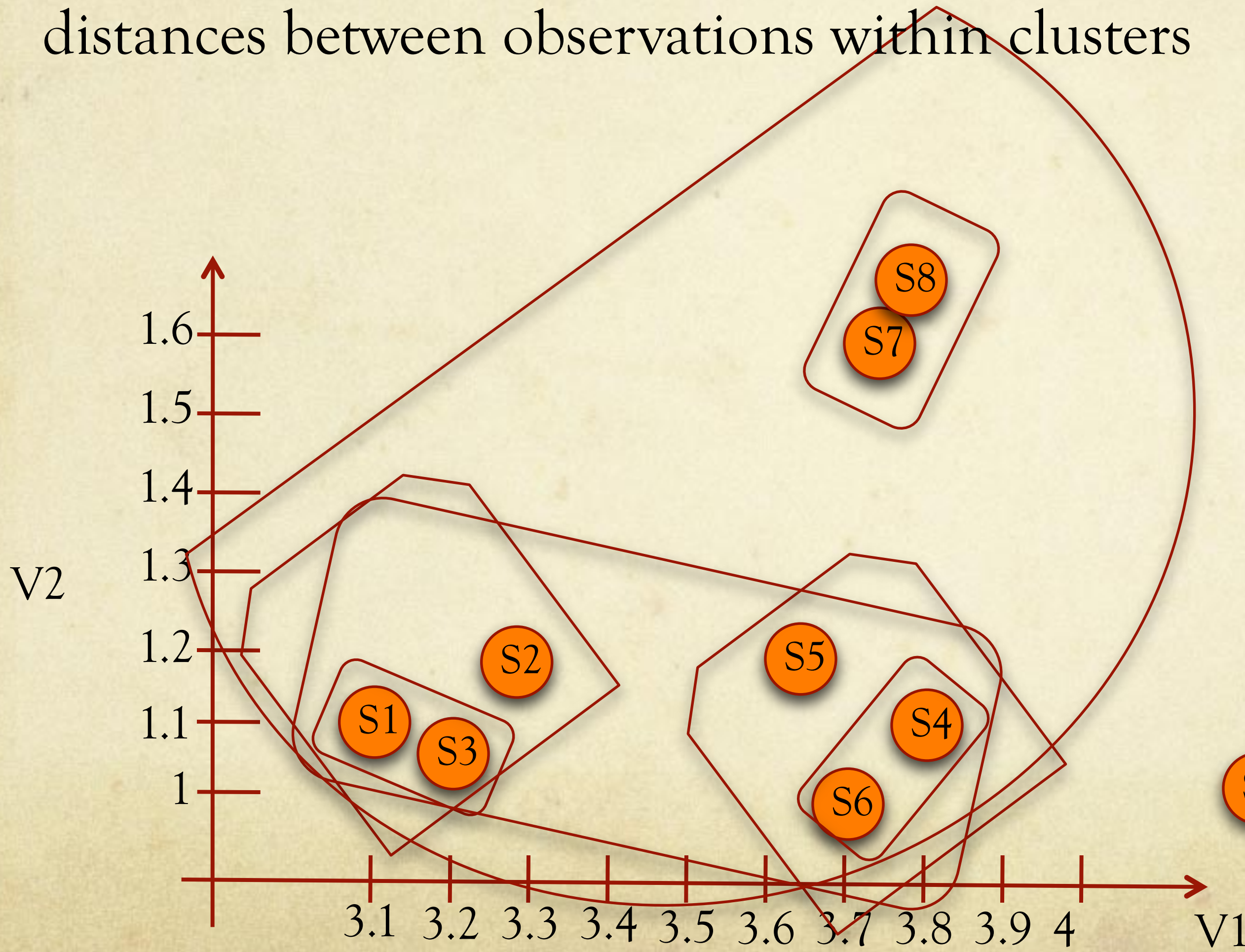
A22: iteratively merge clusters which are more close one to another

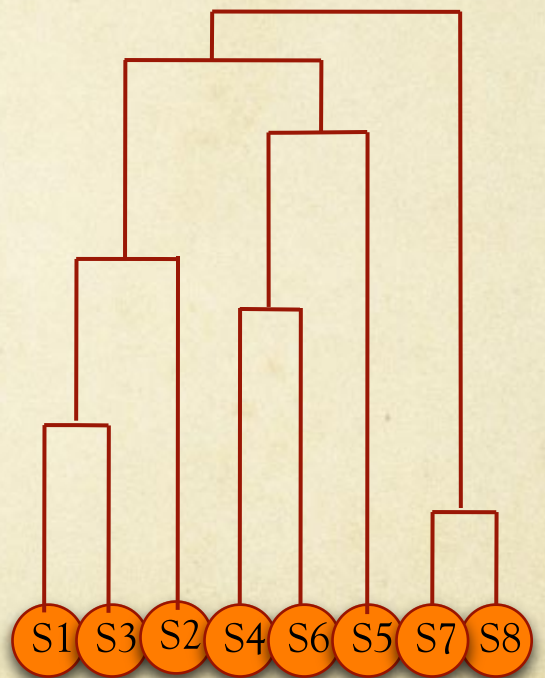


How does it work?

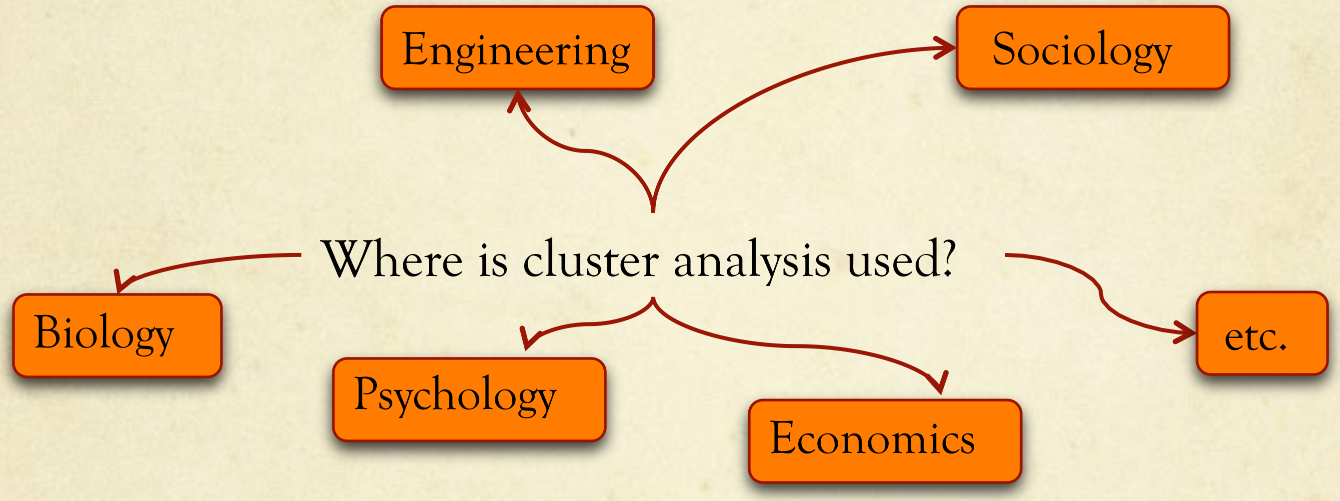
Q3: how to determine the number of clusters in the final solution?

A3: measuring homogeneity of a cluster solution by averaging all distances between observations within clusters





Area of applications



Most common criticisms

Cluster analysis

- is "*descriptive, atheoretical and noninferential*"

- will "*always produce clusters regardless of the actual existence of any structure*"

- "*the cluster solution is not generalisable because it is totally dependent upon the variables used as a basis for the similarity measure*"

Review

- Key elements and notations in *cluster analysis*
- What is cluster analysis and what is not? – difference between *supervised* and *unsupervised* classification
- How it works?
- Research questions addressed by cluster analysis

Cluster Analysis Diagram

Stage 1: Objectives of Cluster Analysis

Stage 2: Research Design Issues

Stage 3: Assumptions in Cluster Analysis

Stage 4: Deriving Clusters and Assessing Overall Fit

Stage 5: Interpreting the Clusters

Stage 6: Validating and Profiling the Clusters

Cluster Analysis – Objectives

Stage 1: Objectives of Cluster Analysis

Select objectives

Select objectives	Taxonomy description	– for exploratory purposes and the formation of a taxonomy (an empirically based classification of objects)
	Data simplification	– a researcher could face a large number of observations that are meaningless unless classified into manageable groups
	Hypothesis generation or testing	– a researcher wishes to develop hypothesis concerning the nature of the data or to examine previously stated hypothesis
	Relationship identification	– a researcher wishes to reveal relationships among observations that are not possible with individual observations

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Five questions to be asked before starting:

1. What variables are relevant?
2. Is the sample size adequate?
3. Can outliers be detected and if so should they be removed?
4. How should object similarity be measured?
5. Should data be standardized?

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Q1: What variables are relevant?

Select clustering variables

Theoretical, conceptual and practical considerations must be observed when selecting variables for clustering analysis

Feature selection methods enable users to select the most relevant variables to be used in cluster analysis

Feature extraction methods enable users to derive new features from the existing features which could be more relevant then the existing features for cluster analysis

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Q2: Is the sample size adequate?

A2: the sample size must be large enough to provide sufficient representation of small groups within the population and represent the underlying structure

Remark - the issue of sample size do not relates to any statistical inference issues

Optimal sample size - the researcher should

- ensure the sample size is sufficiently large to adequately represent all relevant groups
- specify the group sizes necessary for relevance for the questions being asked

Remark:

1. Interest is focus on the identification of small groups – large sample size
2. Interest is focus on the identification of large groups – small sample size

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Q3: Can outliers be detected and if so should they be removed?

What outliers can be?

1. Truly aberrant observation not representative for the population	- distort the actual structure and result in unrepresentative clusters – should be removed
2. Representative observations of small or insignificant groups	- should be removed so that the resulting clusters represent more accurately relevant groups
3. An undersampling of the actual group in the population that causes poor representation of the group	- they represent valid and relevant groups - should be included in the clustering solution

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Q4: How should object similarity be measured?

Three ways to measure inter-objects similarities		
	correlation measures distance measures	require metric data
	association measures	require non-metric data

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Q4: How should object similarity be measured?

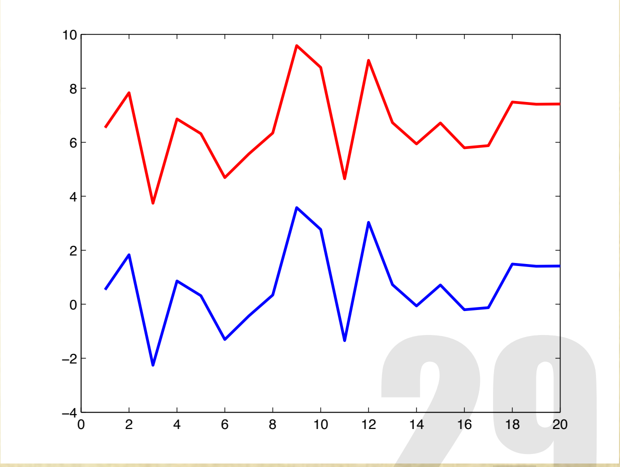
Correlation measures

Pearson's correlation coefficient

$$CC(X_i, X_j) = \frac{\sum_{k=1}^{d}(X_i - \mu_{X_i})(X_j - \mu_{X_j})}{\frac{1}{d-1}\sum_{k-1}^{d}(X_i - \mu_{X_i})\sum_{k=1}^{d}(X_j - \mu_{X_j})}$$

Spectral angle

$$SA(X_i, X_j) = a\cos(CC(X_i, X_j))$$



Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Q4: How should object similarity be measured?

Distance measures

r - metrics

Let $X = \left\{ X_k^n, X_k \in \Re^d \right\}$

then $L_r(X_i, X_j) = \left(\sum_{k=1}^{d} (x_{ik} - x_{jk})^r \right)^{1/r}$

Metric exponent

Minkowski metrics $r \geq 1$

Fractionary metrics $r < 1$

$r = 1$ Manhattan distance

$r = 2$ Euclidian distance

$r \geq 3$ High order metrics

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Q4: How should object similarity be measured?

Distance measures

L_1 - metrics

$$L_r(X_i,X_j) = \left(\sum_{k=1}^{d} (x_{ik} - x_{jk})^r \right)^{1/r}$$

Mahalanobis distance

$$MD(X_i,X_j) = \frac{\sum_{k=1}^{d} (X_i - X_j)}{\frac{1}{d-1}\sum_{k-1}^{d} (X_i - \mu_{X_i}) \sum_{k=1}^{d} (X_j - \mu_{X_j})}$$

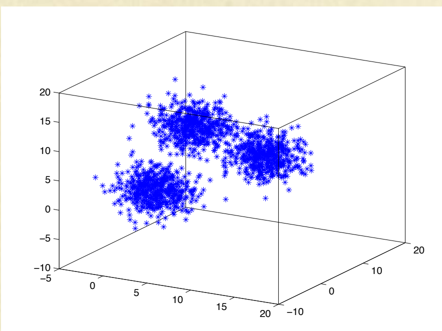
Pearson's correlation coefficient

$$CC(X_i,X_j) = \frac{\sum_{k=1}^{d} (X_i - \mu_{X_i})(X_j - \mu_{X_j})}{\frac{1}{d-1}\sum_{k-1}^{d} (X_i - \mu_{X_i}) \sum_{k=1}^{d} (X_j - \mu_{X_j})}$$

Cluster Analysis – Research design issues

Some clues for metric choice

Should be used when data are dissimilar from the magnitude point of view



Low dimensional spaces – Euclidean distance

High dimensional spaces – Manhatan or fractionary metrics

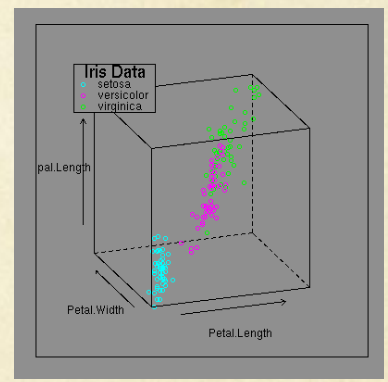
r - metrics

Pearson's correlation coefficient

Spectral angle

Low dimensional spaces – Spectral angle

High dimensional spaces – spectral angle of correlation coefficient



Should be used when data are dissimilar from the correlation point of view

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

Q5: Should data be standardized?

Remark1: Distance measures used to estimate inter-object similarities are sensitive to different scales or magnitudes among the variables.

Remark2: In general, variable with a larger dispersion (standard deviation) will have a bigger impact on the clustering results.

A5: Clustering variables that are not all of the same scale should be standardized.

Cluster Analysis – Research design issues

Stage 2: Research Design Issues

	$Sample_1$	$Sample_2$	$Sample_3$	…
$Variable_1$	$Value_{11}$	$Value_{21}$	$Value_{31}$	
$Variable_2$	$Value_{12}$	$Value_{22}$	$Value_{32}$	
$Variable_3$	$Value_{13}$	$Value_{23}$	$Value_{33}$	
…	⋮	⋮	⋮	

Q5: Should data be standardized?

Standardization techniques:

- Z - score

$$V_i = \frac{V_i - \mu_{V_i}}{\sigma_{V_i}}$$

- Range scaling

$$V_i = \frac{V_i - \min(V_i)}{\max(V_i) - \min(V_i)}$$

- Variable standardization
- Sample standardization

Cluster Analysis – Assumptions

Stage 3: Assumptions in Cluster Analysis

1. It is always assumed that the sample is representative for the population

2. It is assumed that variables are not correlated; if variables are correlated, remove correlated variables or use distance measures that compensates for the correlation such as Mahanalobis distance

Cluster Analysis – Methods

Stage 4: Deriving Clusters and Assessing Overall Fit

Methods:

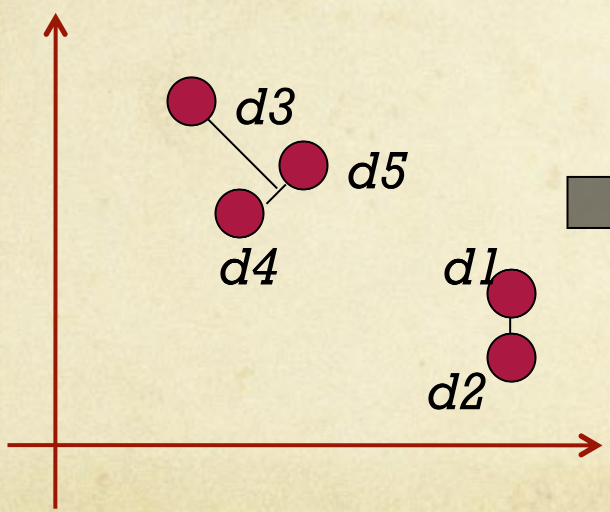
- Hierarchical clustering
  - Agglomerative
  - Divisive
- Partitional clustering
  - K-means
  - Fuzzy K-means
  - Isodata
- Density based clustering
  - Denclust
  - CLUPOT
  - Mean Shift
  - SVC
  - Parzen-Watershed

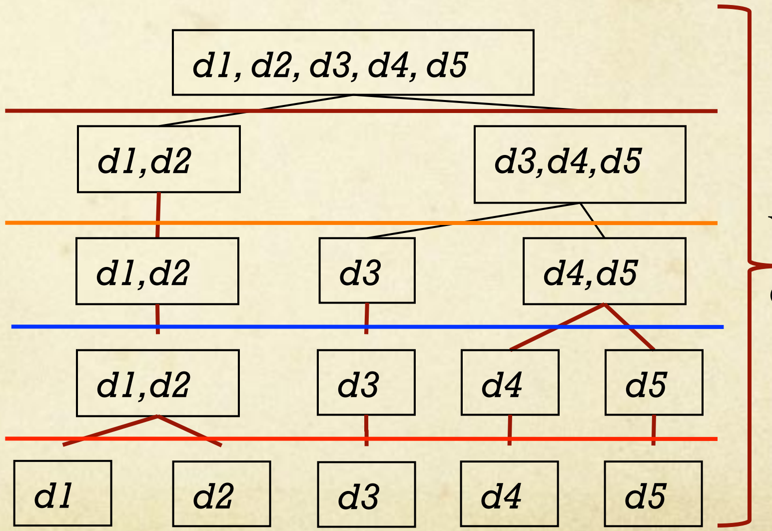
Cluster Analysis – Methods

Hierarchical clustering

Agglomerative (bottom - up)

Principle: compute the Distance-Matrix between all objects (initially one object = one cluster). Find the two clusters with the closest distance and put those two clusters into one. Compute the new Distance-Matrix.





Where to cut dendogram?

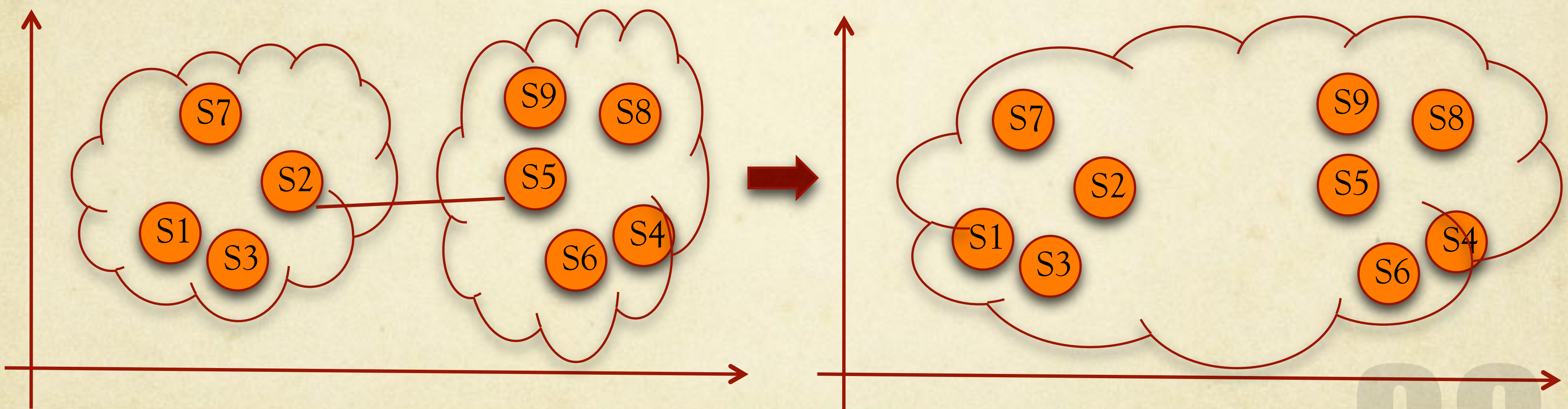
Cluster Analysis – Methods

Hierarchical clustering

Agglomerative (bottom - up)

Single-link (nearest neighbor method)

$$sim(c_i, c_j) = \min_{x \in c_i, y \in c_j} sim(x, y)$$

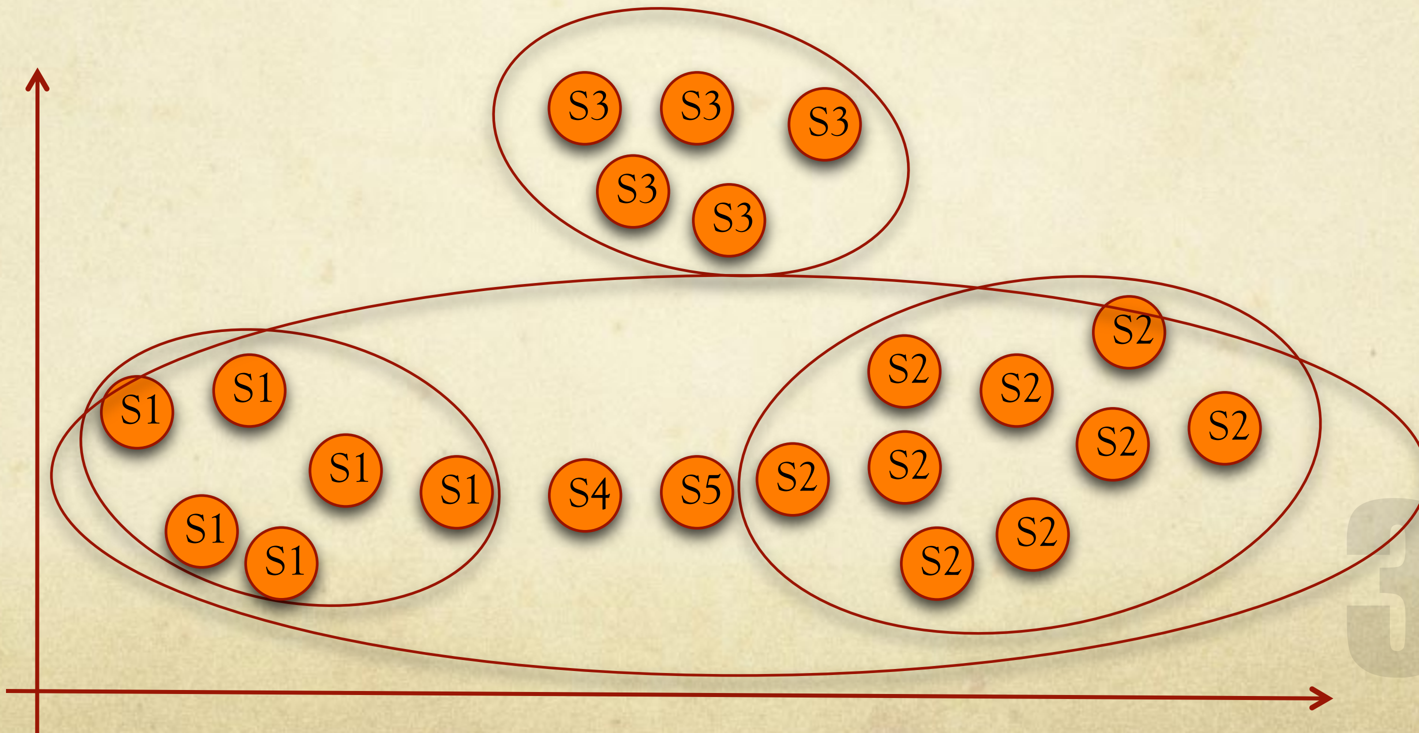


Drawback: can result in long and thin clusters due to chaining effect

Cluster Analysis – Methods

Single-link (nearest neighbor method)

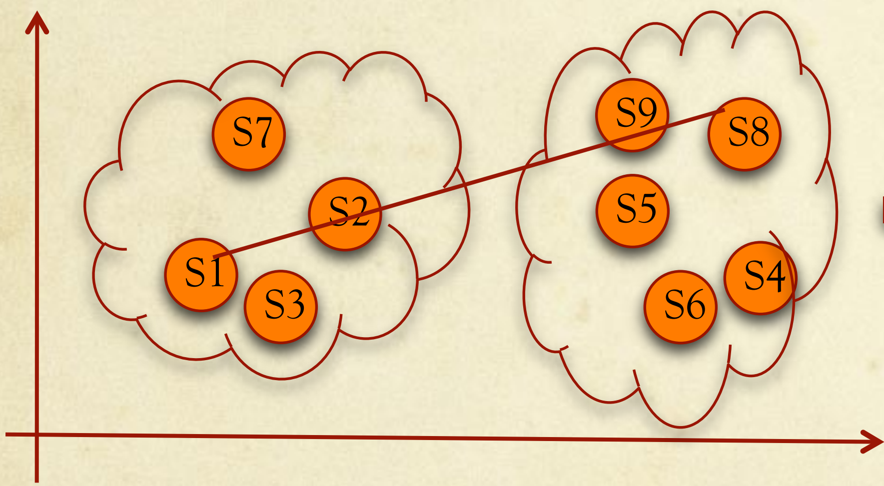
Drawback: can result in long and thin clusters due to chaining effect

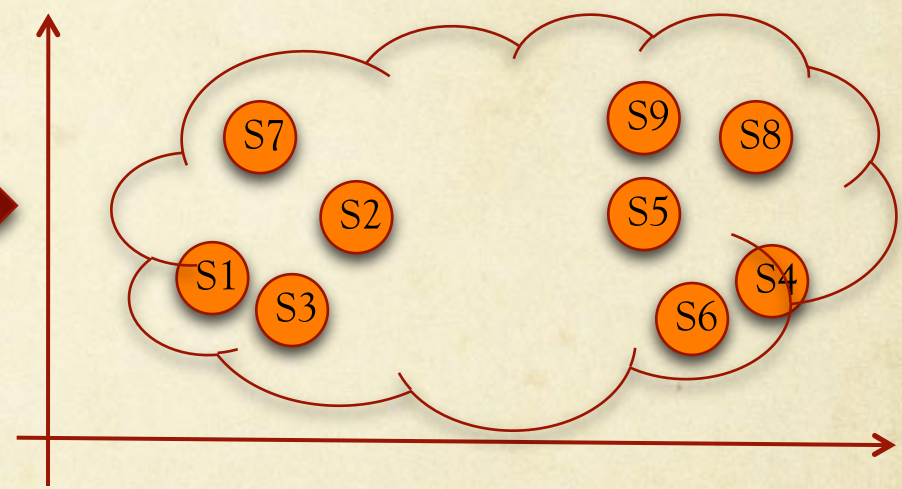


Cluster Analysis – Methods

Complete-linkage (furthest-neighbor or diameter method)

$$sim(c_i, c_j) = \max_{x \in c_i, y \in c_j} sim(x, y)$$



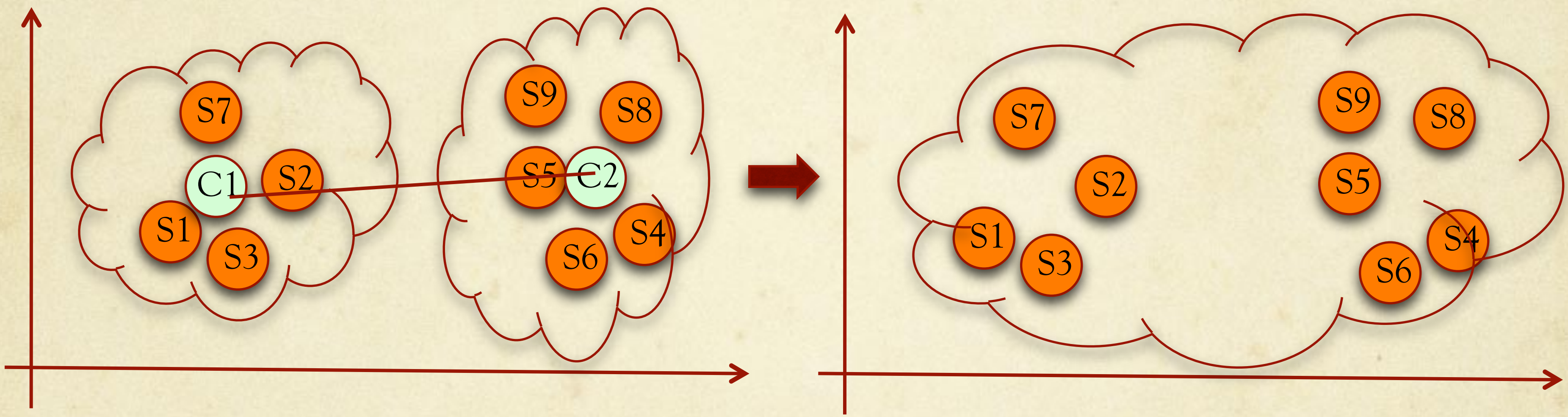


Drawback: makes spherical clusters

Cluster Analysis – Methods

Average-linkage (Centroid method)

Similarity between clusters is the average distance between all objects in one cluster and all objects in other cluster



Advantage: less affected by outliers

Drawback: generates clusters with approximately equal within cluster variation

Cluster Analysis – Methods

Divisive (top-down)	- divisive algorithms need much more computing power so in practical only agglomerative methods are used
Computational complexity	- $O(n^2)$ - optimal
Drawbacks	- computation of similarity matrix between all pairs of points; for large datasets this is computational expensive

Cluster Analysis – Methods

Partitional clustering

- A typical clustering analysis approach via partitioning data set iteratively
- Statement of the problem: given a K, find a partition of K *clusters* to optimize the chosen partitioning criterion
- In principle, partitions achieved via minimizing the sum of squared distances in each cluster

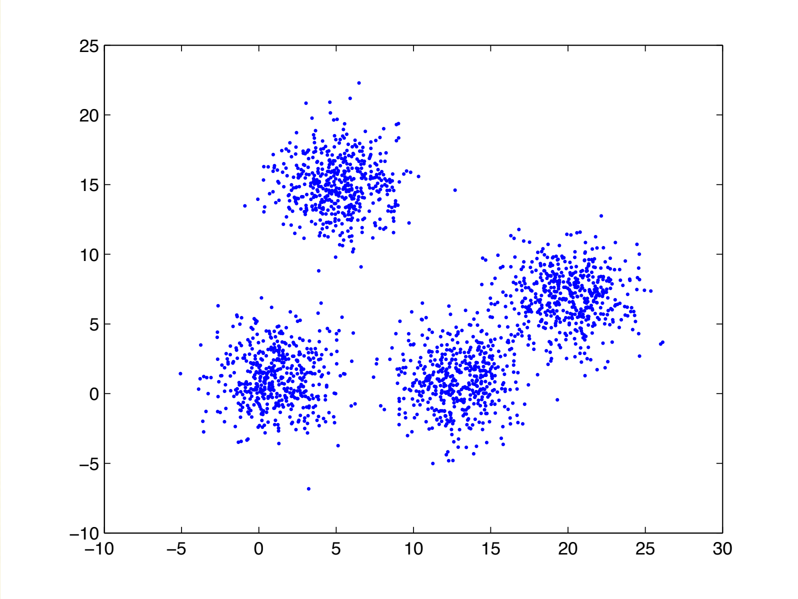
$$E = \Sigma_{i=1}^{K} \Sigma_{\mathbf{x} \in C_i} \| \mathbf{x} - \mathbf{m}_i \|^2$$

K-means - (MacQueen'67): each cluster is represented by the centre of the cluster and the algorithm converges to stable centers of clusters

Cluster Analysis – Methods

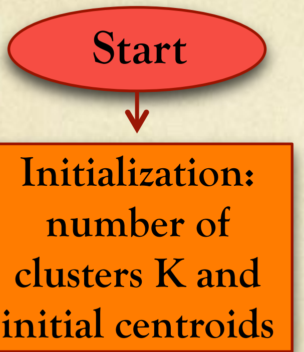
K-means algorithm

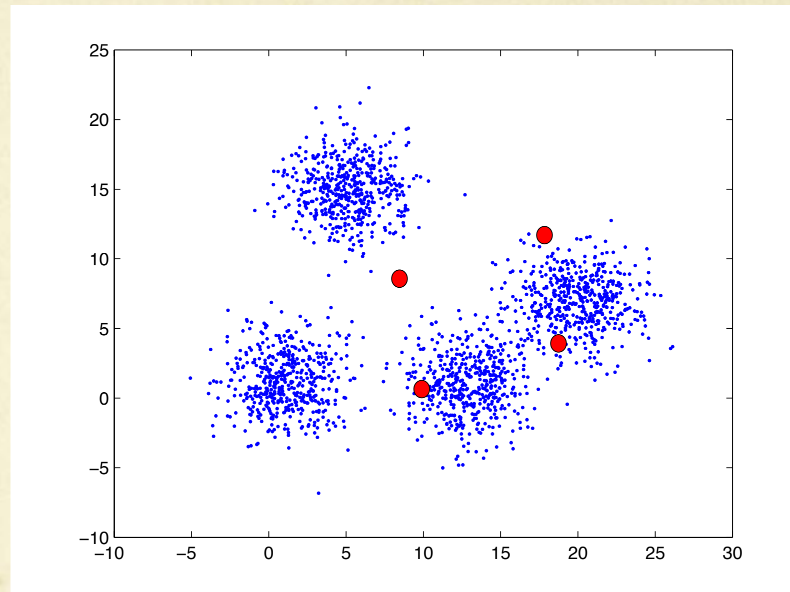
Start



Cluster Analysis – Methods

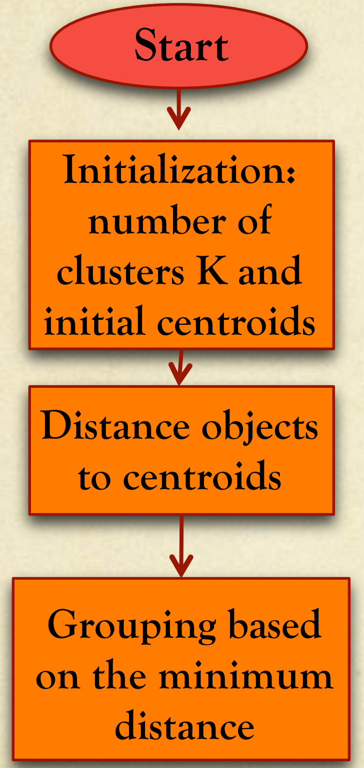
K-means algorithm

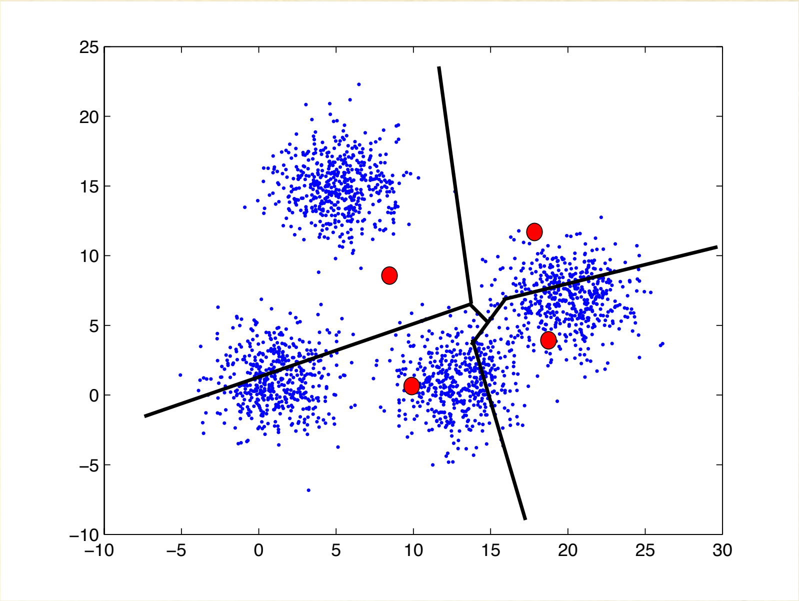




Cluster Analysis – Methods

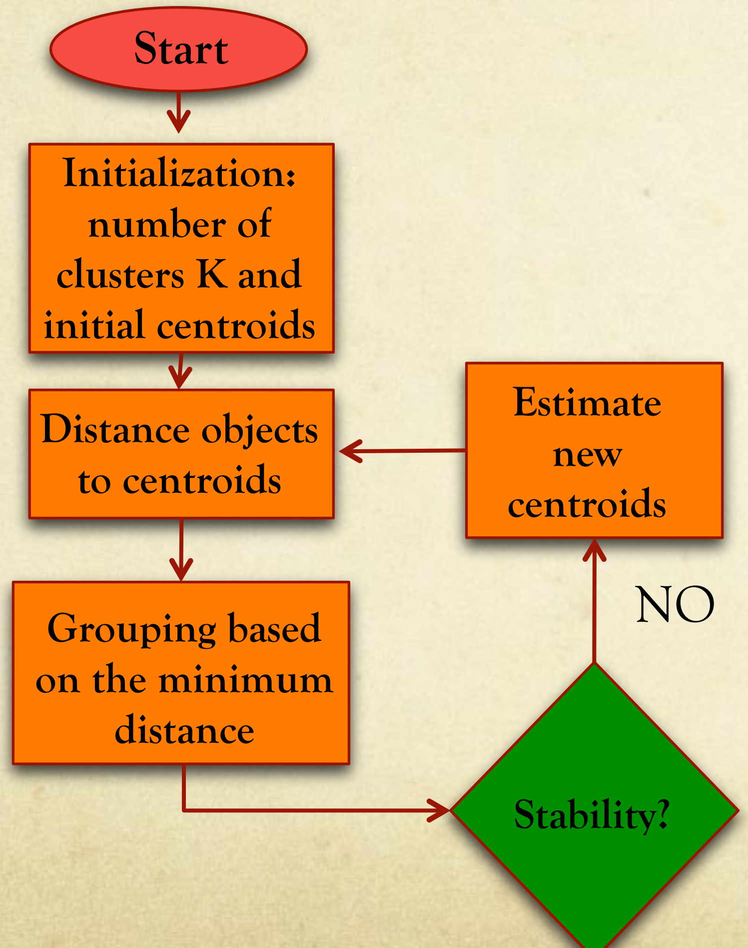
K-means algorithm

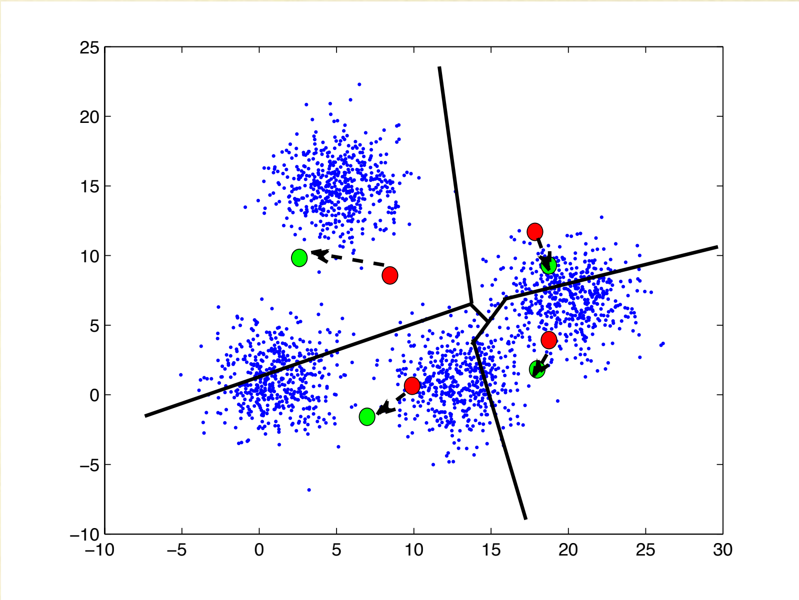




Cluster Analysis – Methods

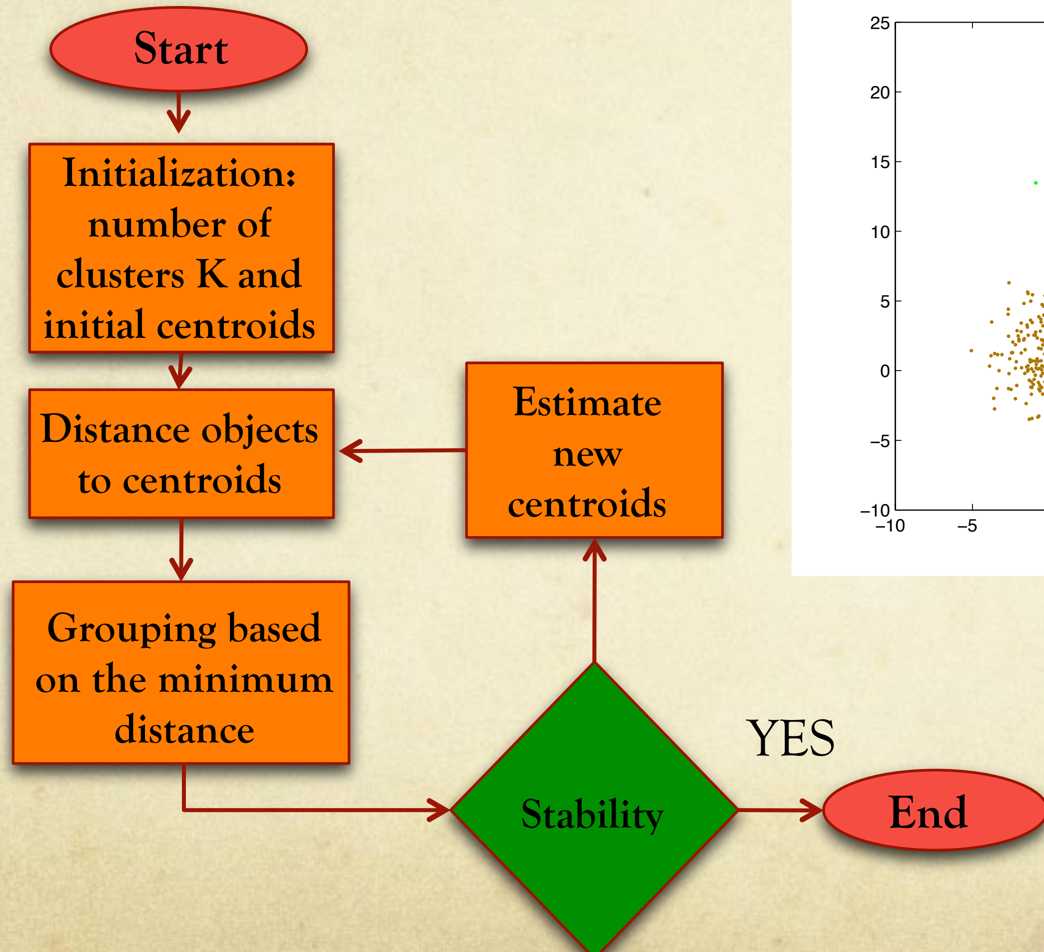
K-means algorithm

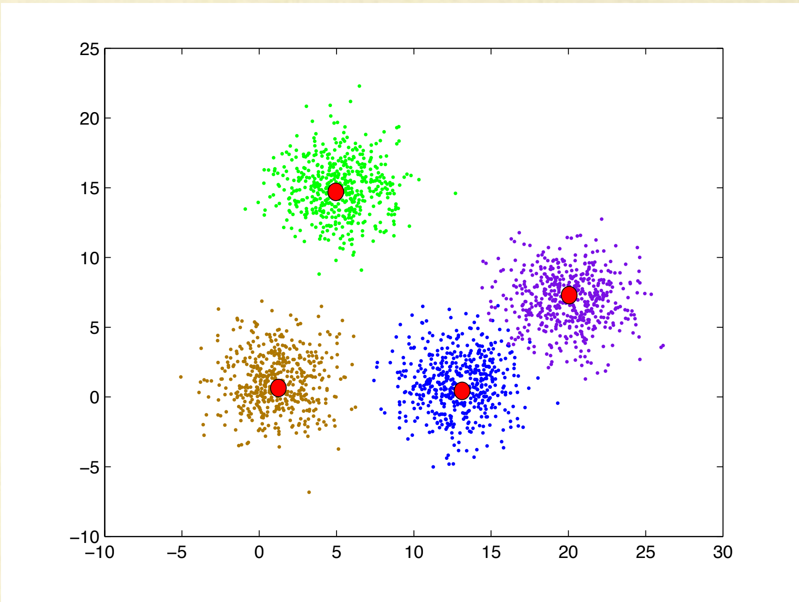




Cluster Analysis – Methods

K-means algorithm



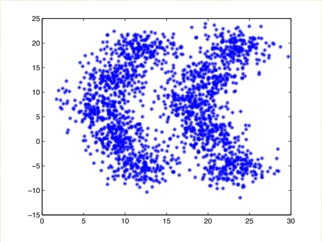


Cluster Analysis – Methods

Drawbacks

Sensitive to initial seed points

Converge to a local optimum that may be unwanted solution



Need to specify K, the *number* of clusters, in advance

Unable to handle noisy data and outliers

Not suitable for discovering clusters with non-convex shapes

Applicable only when mean is defined, then what about categorical data?

Advantages

Efficient in computation

$O(tKn)$, where n is number of objects, K is number of clusters, and t is number of iterations. Normally, K, $t << n$

Cluster Analysis – Methods

Density based clustering

- Clustering based on density (local cluster criterion), such as density-connected points or based on an explicitly constructed density function
- Major features
  - Discover clusters of arbitrary shape
  - Handle noise (outliers)

DBSCAN - Ester, et al. 1996 - http://www2.cs.uh.edu/~ceick/7363/Papers/dbscan.pdf

DENCLUE - Hinneburg & D. Keim 1998 - http://www2.cs.uh.edu/~ceick/7363/Papers/dbscan.pdf

Parzen Watershed - http://www.ecmjournal.org/journal/smi/pdf/smi97-01.pdf

MeanShift - http://courses.csail.mit.edu/6.869/handouts/PAMIMeanshift.pdf

Support Vector Clustering - http://jmlr.csail.mit.edu/papers/volume2/horn01a/rev1/horn01ar1.pdf

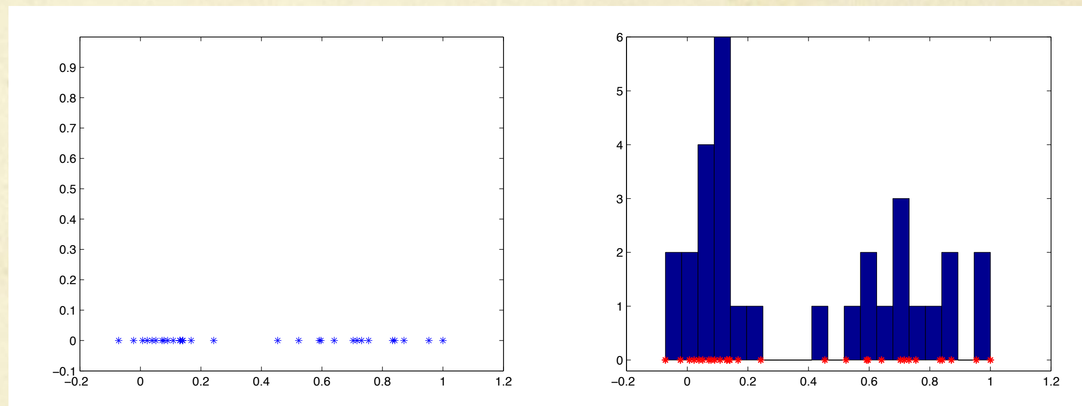
Cluster Analysis – Methods

Density is the number of points within a specified space range

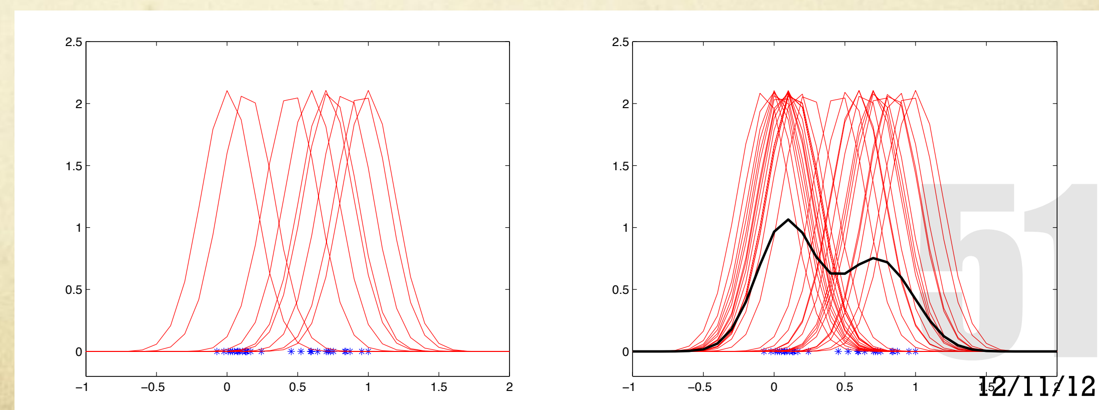
Density estimation

An example on univariate data

From histograms...



...to kernel density estimation
(Parzen window technique)



$$f(x) = \sum_i K(x - x_i) = \sum_i k\left(\frac{\|x - x_i\|^2}{h^2}\right)$$

$k(r)$ - kernel function or parzen window

Cluster Analysis – Methods

Why is density estimation computational expensive in high dimensional spaces?

$$f(x) = \sum_i K(x - x_i) = \sum_i k\left(\frac{\|x - x_i\|^2}{h^2}\right)$$

$k(r)$ - kernel function or parzen window

S – discrete space 1D with n = 10 discrete values

S2 – discrete space 2D with n^2 discrete values

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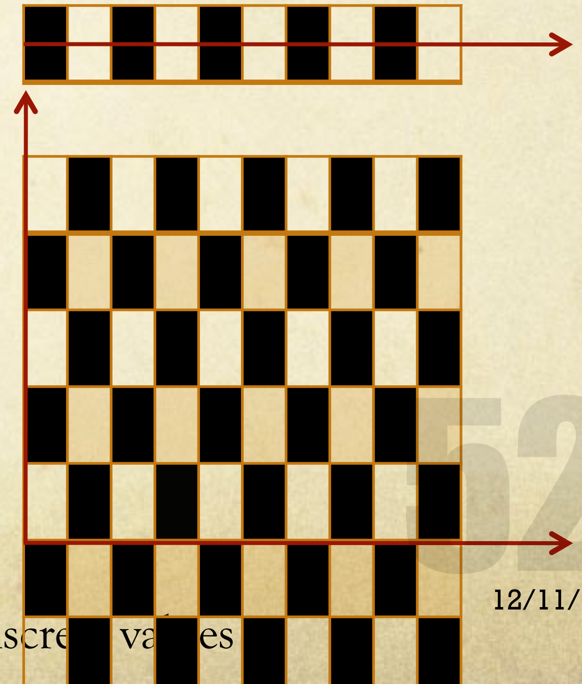
S10 – discrete space 2D with n^10 = 10.000.000.000 discrete values

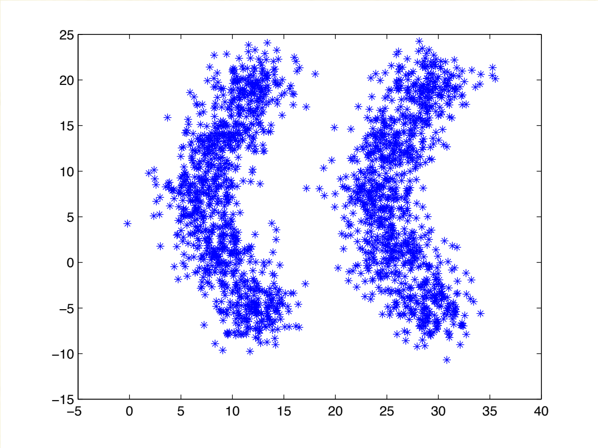


Parzen Watershed algorithm

In based on the density estimation of the *pdf* in the feature space

Algorithm

Start → Dimension reduction



Parzen Watershed algorithm

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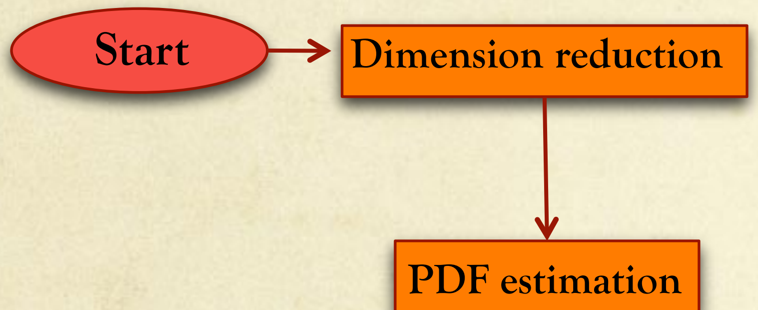
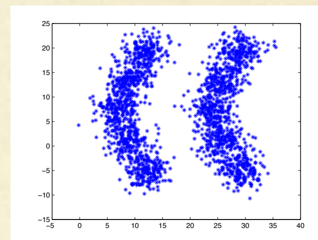
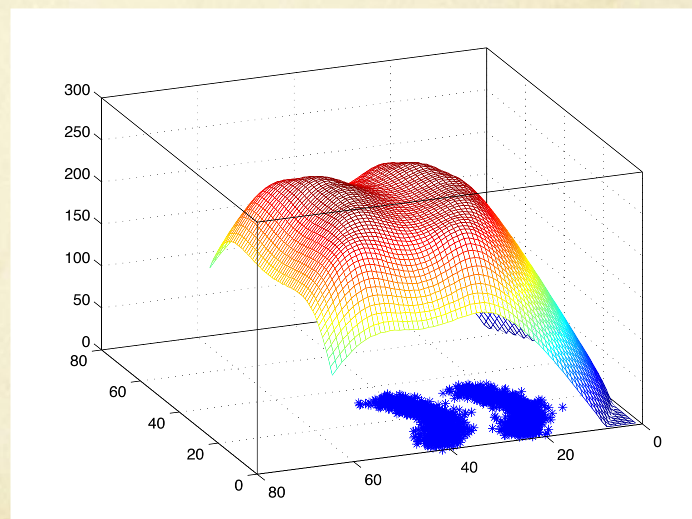






Parzen Watershed algorithm

In based on the density estimation of the *pdf* in the feature space

Algorithm

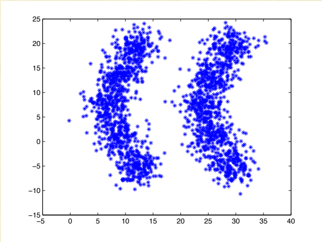
Start → Dimension reduction

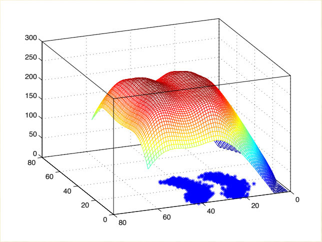
↓

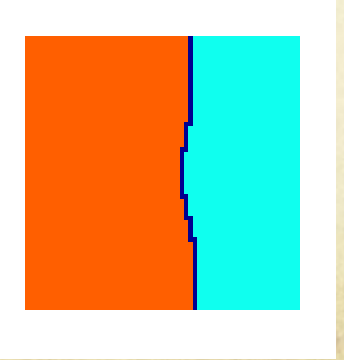
PDF estimation

↓

Split feature space into influence zones







Parzen Watershed algorithm

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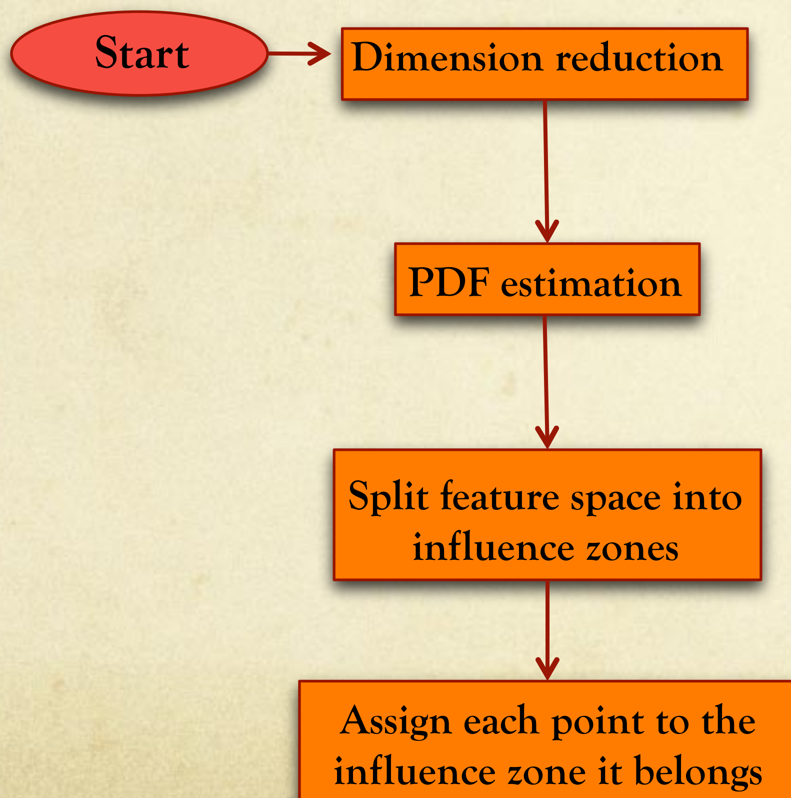
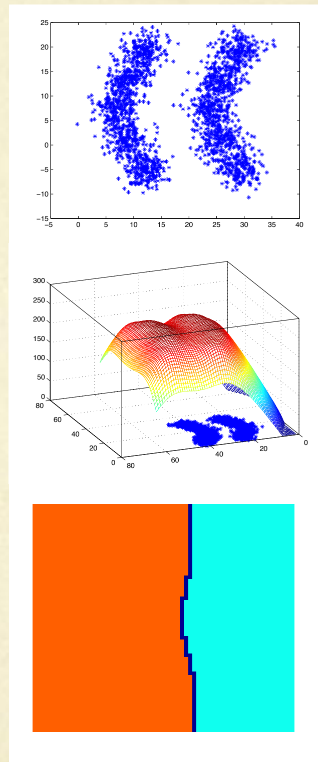
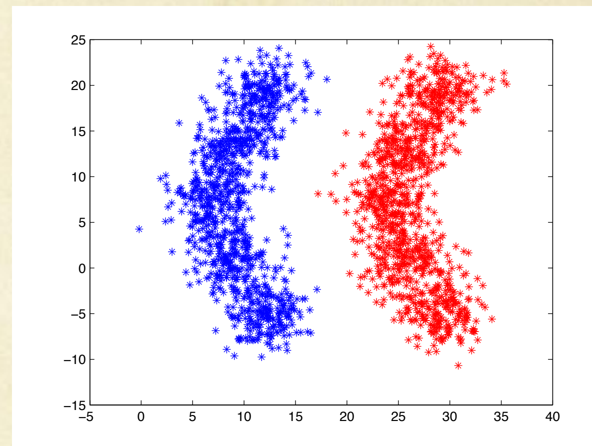






Parzen Watershed algorithm

Strengths :

- Application independent tool
- Suitable for real data analysis
- Does not assume any prior shape (e.g. elliptical) on data clusters
- Can handle arbitrary feature spaces
- Only ONE parameter to choose
- *H (window size) has a physical meaning, unlike K-Means*

Weaknesses :

- The window size (bandwidth selection) is not trivial
- Inappropriate window size can cause modes to be merged, or generate additional "shallow" modes -> Use adaptive window size
- Low dimension feature space
- Computational complexity high

Cluster Analysis – Interpreting the clusters

Stage 5: Interpreting the clusters

The cluster centroid (a mean profile of the cluster on each cluster variable) is particularly useful in the interpretation stage

Interpretation involves:

- Examining and distinguishing characteristics of each cluster's profile and identifying substantial differences between clusters
- Cluster solution failing to reveal significant differences indicate that other solutions should be examined
- The cluster centroid should also be assessed for correspondence to researcher's prior expectation based on theory or practical experience

Cluster Analysis – Validation

Stage 6: Validating and Profiling the Clusters

"The validation of clustering structures is the most difficult and frustrating part of cluster analysis.
Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage."

Algorithms for Clustering Data, Jain and Dubes

1. Determining the clustering tendency of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
3. Evaluating how well the results of a cluster analysis fit the data *without reference to external information.- Use only the data*
4. *Comparing the results of two different sets of cluster analyses to determine the stability of the solution.*
5. *Determining the 'correct' number of clusters.*

Cluster analysis – Validation

Indices for cluster validation

- Cross validation
- External index – used to measure the extent to which cluster labels match externally supplied class labels
  - Labels provided by experts or ground truth
- Internal index – based on the intrinsic content of the data. Used to measure the goodness of a clustering structure *without respect to external information*
  - Davies Bound – index , Dunn – index, C – index, Silhouette coefficient etc.
- Relative index – used to compare the results of different clustering algorithms
  - Internal or external indices

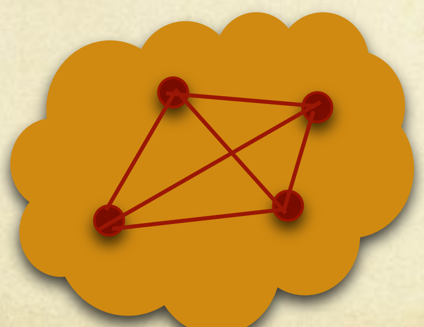
Cluster analysis – Validation

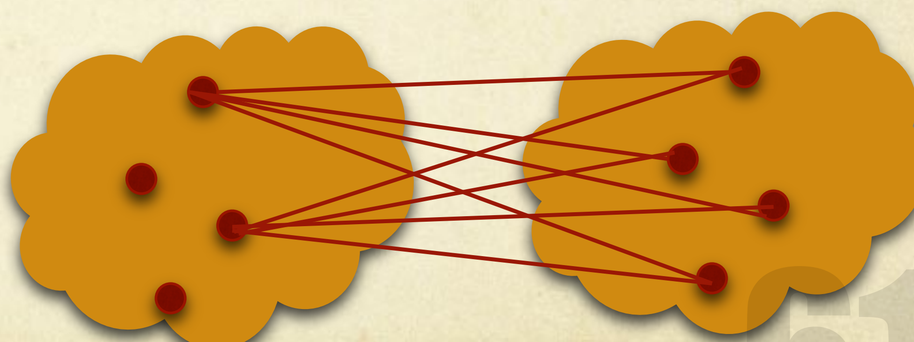
Internal indices – example: silhouette coefficient

$$sc = 1 - \frac{c}{s}$$

Cluster cohesion is the mean value of the distances of all pairs of points within a cluster

Cluster separation is the mean value of the distances between the points in the cluster and points outside the cluster





c – the smallest the better

s – biggest the better

Cluster validation

- K – means, hierarchical
  - Davies Bound – index , Dunn – index, C – index, Silhouette coefficient etc.
- Density based clustering
  - Stability of the number of classes

$$No\_Of\_Classes = f(h)$$

h - window size

Applications

A good way to test random hypothesis (hierarchical and density based clustering)

Image analysis

Medical imaging

Remote sensing imaging

Microscopy imaging

For border detection and object recognition

Character recognition

Computational biology and bioinformatics

Information retrieval

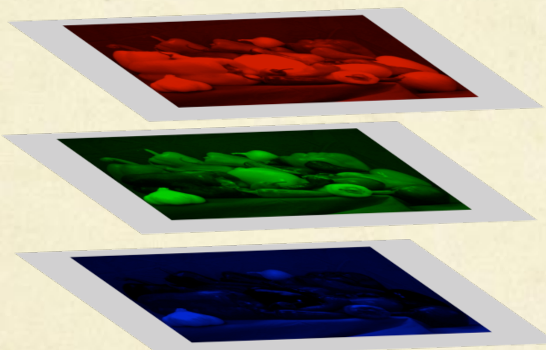
Database segmentation

Web search engines based on clustering – Clusty

Cluster analysis – application to image segmentation

Data

Features



Stage 1: Objectives of Cluster Analysis

Stage 2: Research Design Issues

Stage 3: Assumptions in Cluster Analysis

Stage 4: Deriving Clusters and Assessing Overall Fit

Stage 5: Interpreting the Clusters

Stage 6: Validating and Profiling the Clusters

Cluster analysis – application to image segmentation

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Stage 1: Objectives of Cluster Analysis

Select objectives

- Taxonomy description
- Data simplification
- Relationship identification
- Hypothesis generation or testing

Cluster analysis – application to image segmentation

Stage 1: Objectives of Cluster Analysis

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Stage 2: Research Design Issues

Five questions to be asked before starting:

1. What variables are relevant?
2. Is the sample size adequate?
3. Can outliers be detected and if so should they be removed?
4. How should object similarity be measured?
5. Should data be standardized?

Cluster analysis – application to image segmentation

Stage 1: Objectives of Cluster Analysis

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Stage 3: Assumptions in Cluster Analysis

1. It is always assumed that the sample is representative for the population

2. It is assumed that variables are not correlated; if variables are correlated, remove correlated variables or use distance measures that compensates for the correlation such as Mahanalobis distance

Cluster analysis – application to image segmentation

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Hierarchical clustering

Partitional clustering

Density based clustering

12/11/12

Cluster analysis – application to image segmentation

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12/11/12

Cluster analysis – application to image segmentation

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Stage 6: Validating and Profiling the Clusters

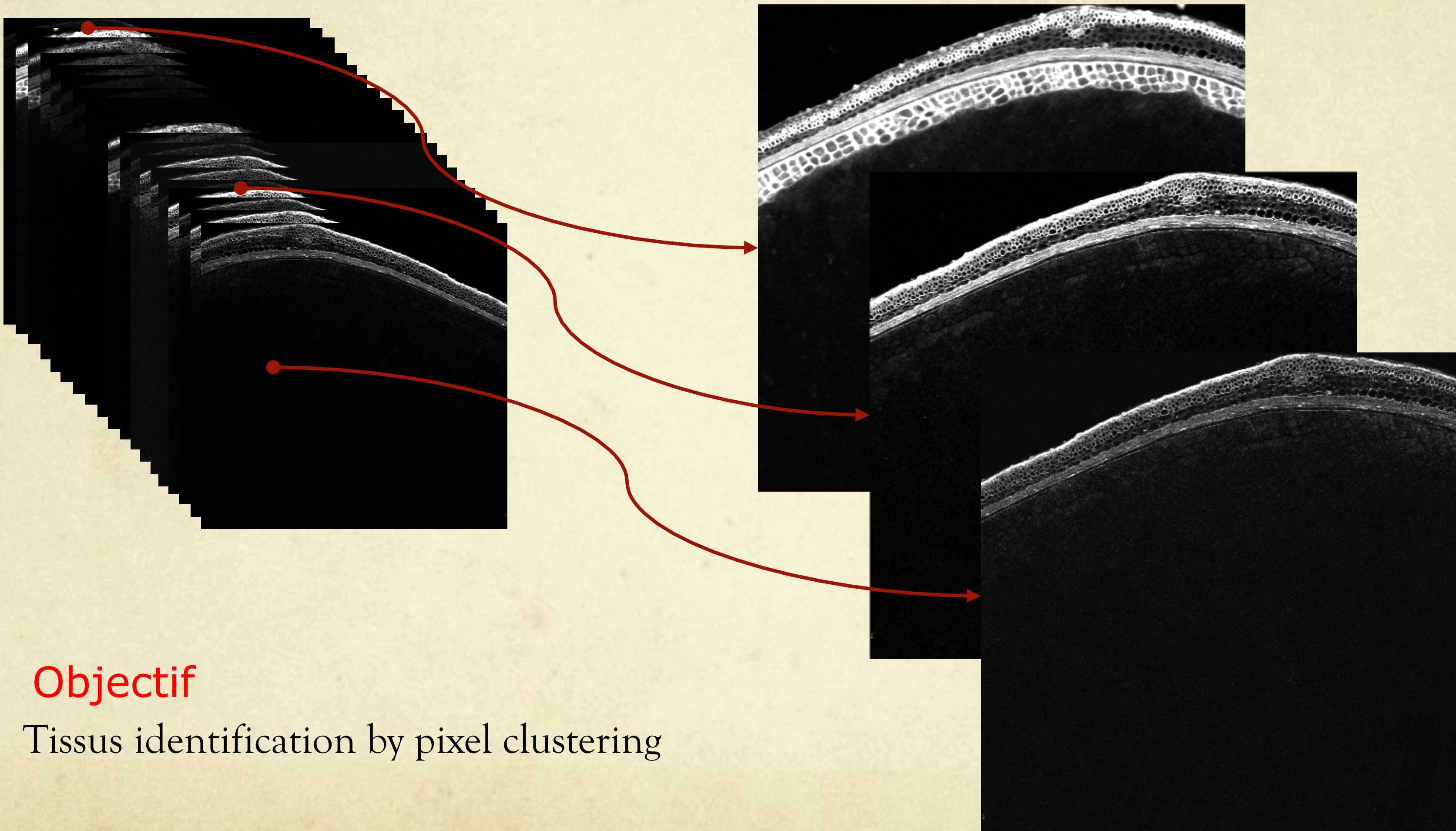
- Cross validation
- External index - labels provided by experts or ground truth
- Internal index
- Relative index

12/11/12

Cluster analysis – application to image segmentation

12/11/12

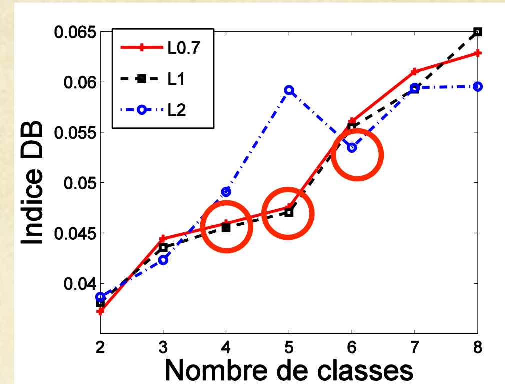
Microscopy imaging



Objectif

Tissus identification by pixel clustering

Application – results



Choosing the optimal metric– indice DB

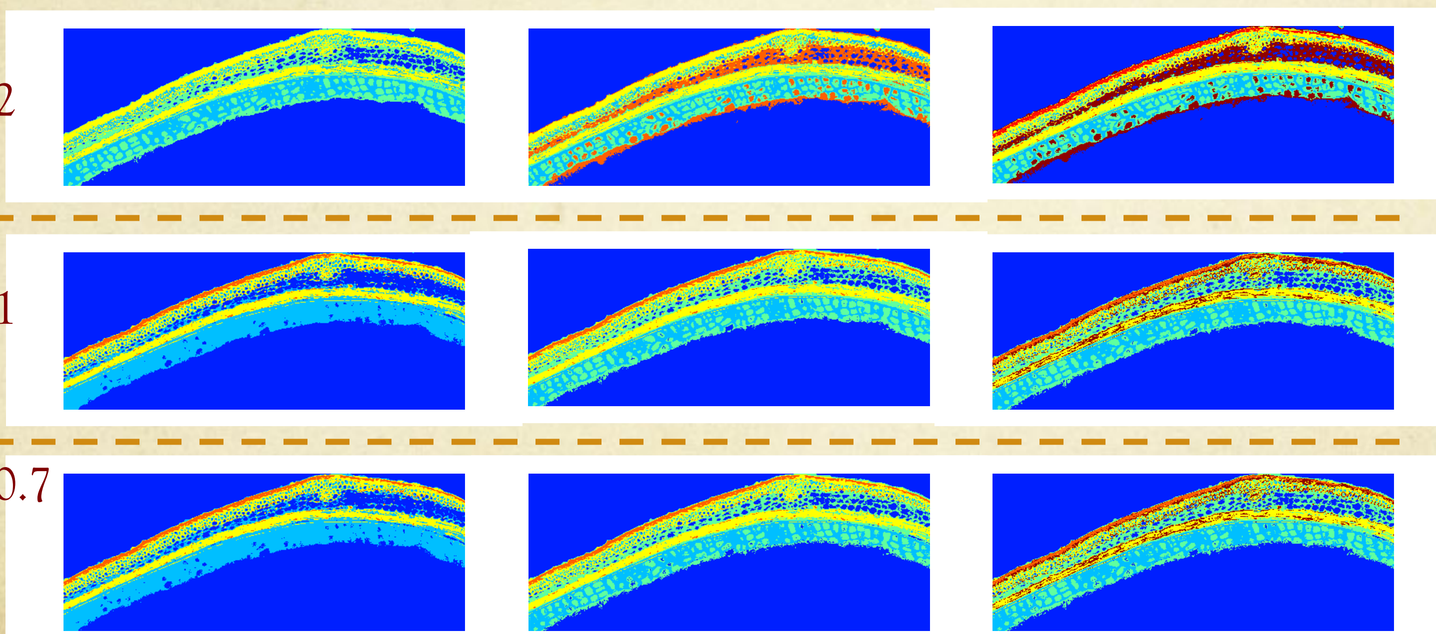
For a fixed K, the minimal value of DB index reveals the most discriminate metric

4 classes 5 classes 6 classes

L2

L1

L0.7

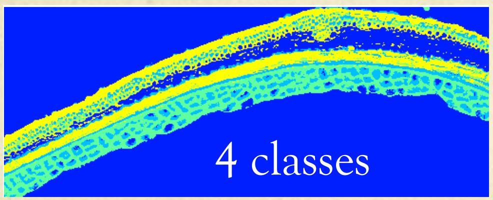


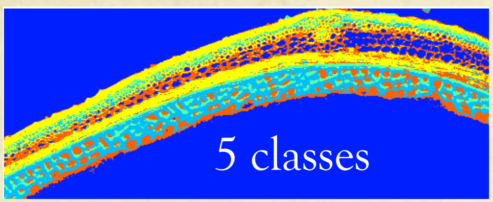
- Background
- Reject class
- Ferulic acid
- Ferulic acid
- Lignin
- Cutin

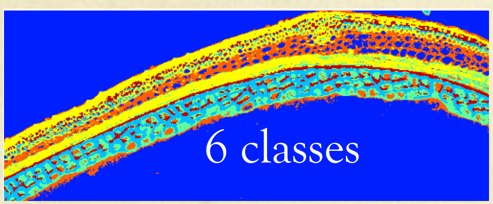
Application – results

Dimension reduction has been performed by NMF

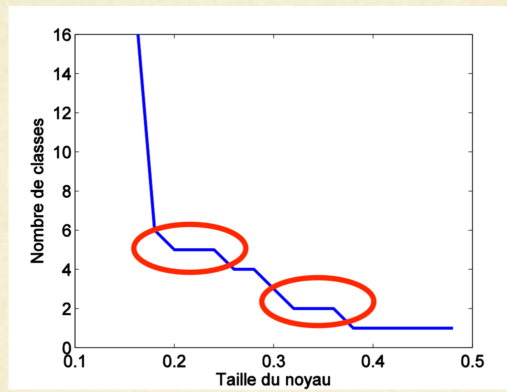
K-means

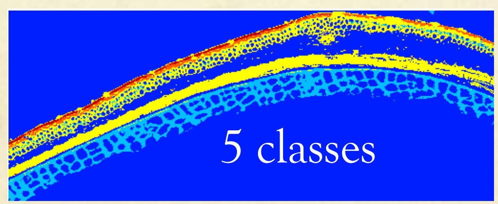




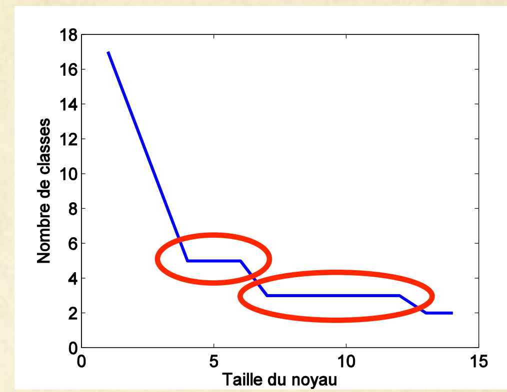


Mean-Shift

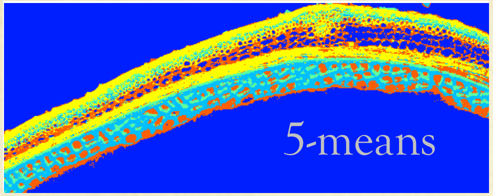


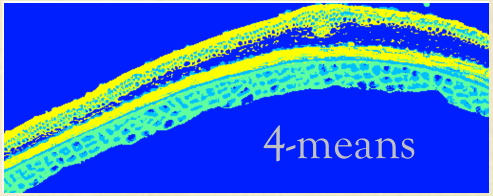


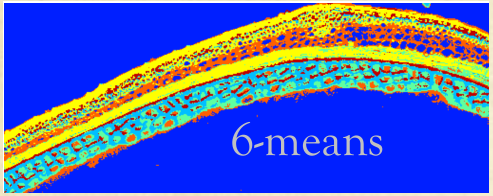
Parzen-Watershed

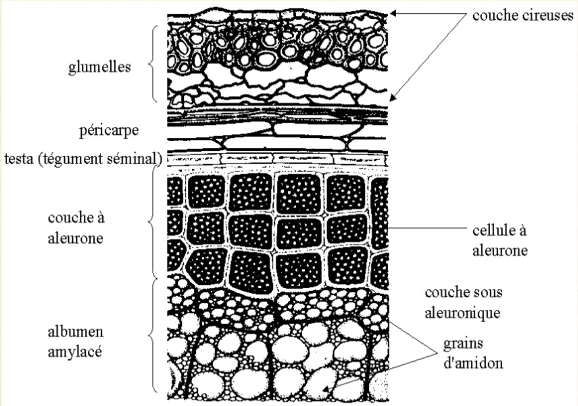


Application – validation of results

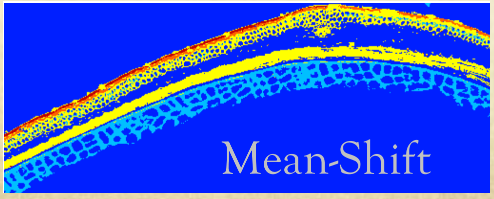








coupe transversale d'un grain d'orge(GASSNER, 1973)



Open questions

High dimensional data…

Which similarity measure???

Recent works have shown that Euclidean distance is meaningless as similarity measure in high dimensional space

Clustering validation???

Most internal indices are designed for convex shape clusters!!!

Bibliography

Joseph F. Hair Jr., Willim C. Black, Barry J. Babin, Rolph E. Anderson- *Multivariate Data Analysis – a global perspective*

Mean shift algorithm

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- Does not assume any prior shape (e.g. elliptical) on data clusters
- Can handle arbitrary feature spaces
- Only ONE parameter to choose
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Weaknesses :

- The window size (bandwidth selection) is not trivial
- Inappropriate window size can cause modes to be merged, or generate additional "shallow" modes -> Use adaptive window size
- For high dimensional data computational expensive

Example:
d – 10, n – 102400
Time = 3837.488139 seconds