Ludwig Maximilians Universität München
Institut für Informatik
Lehr- und Forschungseinheit für Datenbanksysteme

Skript zur Vorlesung

Datenbanksysteme

im Wintersemester 2013/14

Kapitel 12: Clustering

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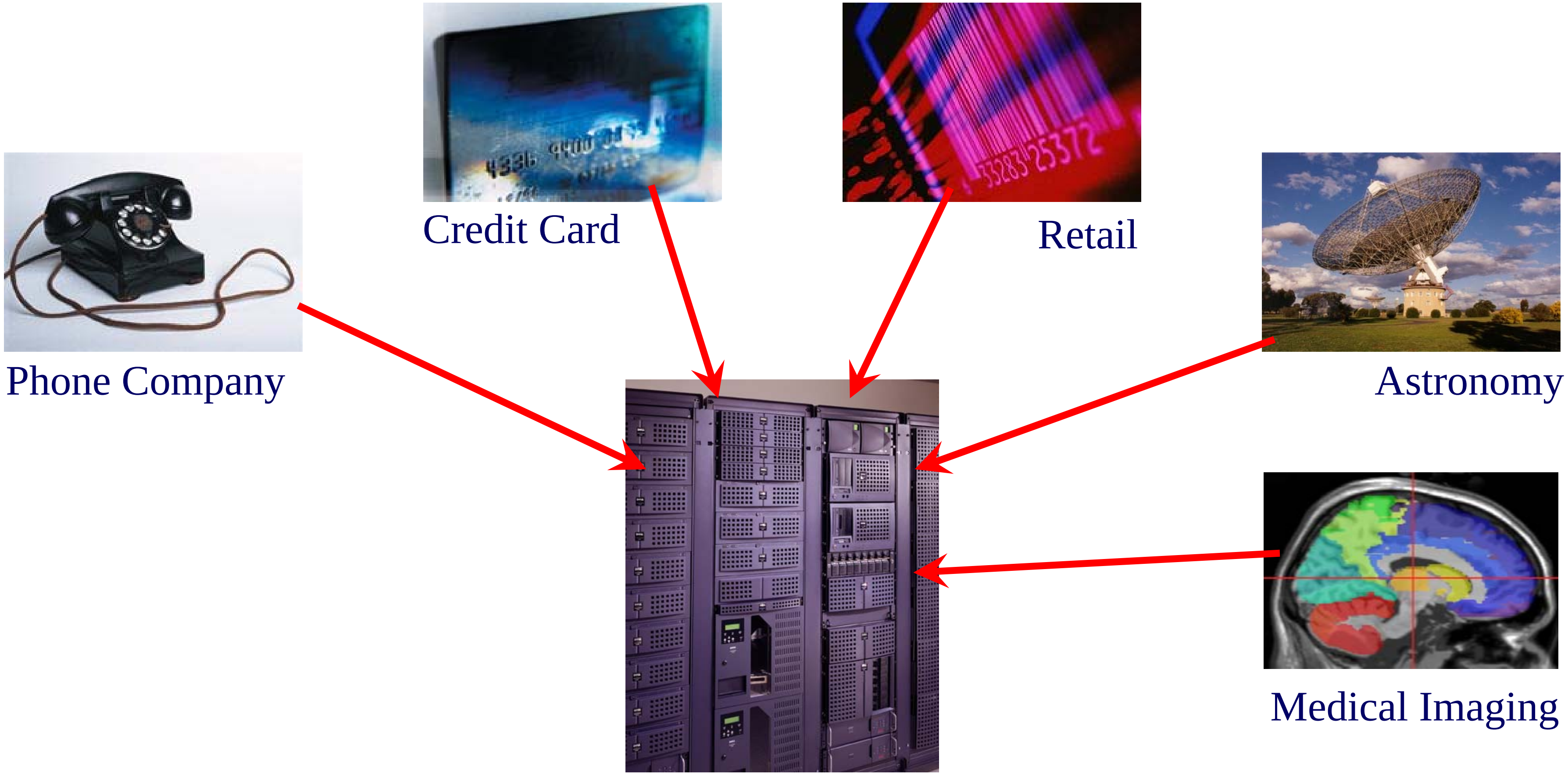
http://www.dbs.ifi.lmu.de/Lehre/DBS

Motivation



- Big data sets are collected in databases
- Manual analysis is no more feasable

Big Data

- The buzzword "Big Data" dates back to a report by McKinsey (May 2011) (http://www.mckinsey.com/insights/business_technology/big_data_the_next_frontier_for_innovation)

- "The amount of data in our world has been exploding, and analyzing large data sets—so-called big data—will become a key basis of competition, underpinning new waves of productivity growth, innovation, and consumer surplus […]"

- "Data have swept into every industry and business function and are now an important factor of production, alongside labor and capital"
  - Potential Revenue in US Healthcare: > $300 Million
  - Potential Revenue in public sector of EU: > €100 Million

- "There will be a shortage of talent necessary for organizations to take advantage of big data. By 2018, the United States alone could face a shortage of 140,000 to 190,000 people with deep analytical skills as well as 1.5 million managers and analysts with the know-how to use the analysis of big data to make effective decisions."

Big Data

- Data Mining is obviously an important technology to cope with Big Data

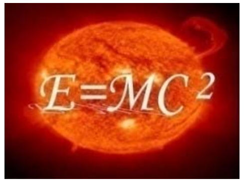
- Caution: “Big Data” does not only mean “big”

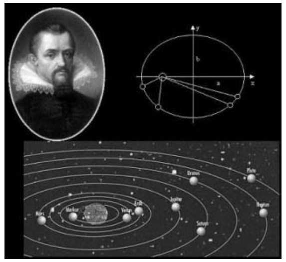
  => Three V’s (the three V’s characterizing big data)

  – Volume	Many objects but also huge represenations of single objects
  – Velocity	Data arriving in fast data streams
  – Variety	Not only one type of data, but different types, semi- or unstructured

A Paradigm Shift in Science?

- Some 1,000 years ago, science was empirical (describing natural phenomena)
- Last few hundred years, science was theoretical (Models, generalizations)





- Last few decades, science became computational (data intensive)
  - Computational methods for simulation
  - Automatic data generation, high-throughput methods, …

- Data Sciene

Definition KDD

[Fayyad, Piatetsky-Shapiro & Smyth 1996]

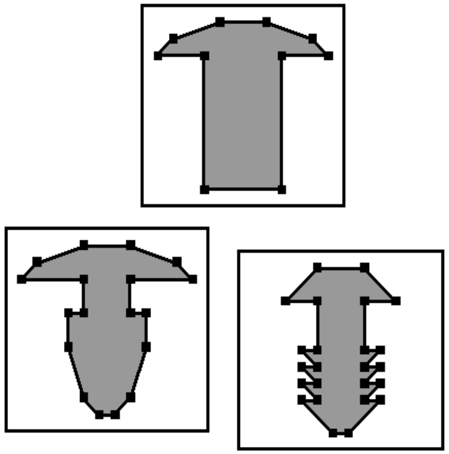
„*Knowledge Discovery in Databases* (*KDD*) is the nontrivial process of identifying patterns in data which are

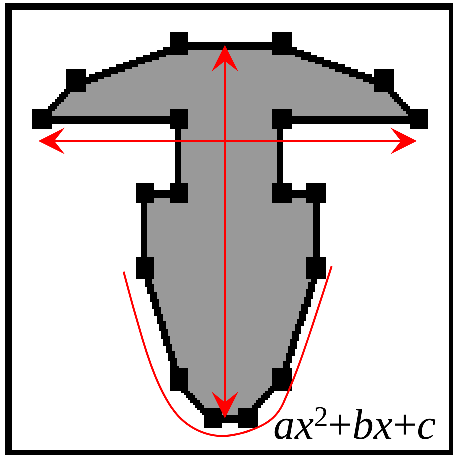
- valid
- novel
- potentially useful
- and ultimately understandable“

Feature Vectors Associated to Objects

- Objects of an application are often complex
- It is the task of the KDD expert to define or select suitable features which are relevant for the distinction between various objects

Example: CAD-drawings:

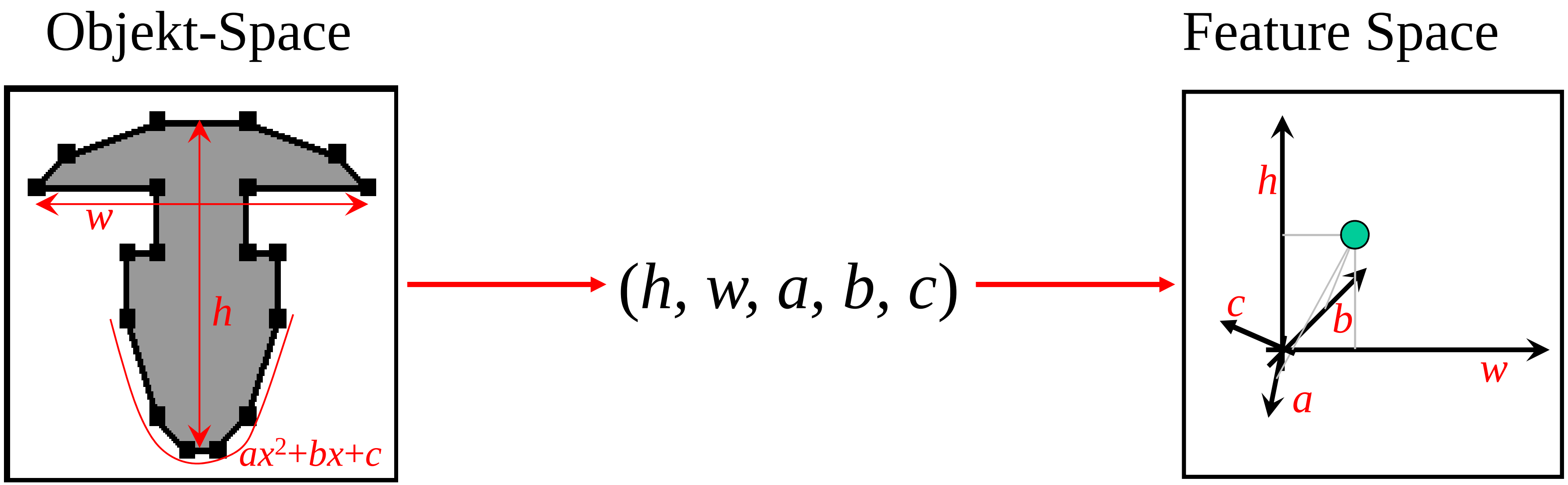




Possible features:

- height h
- width w
- Curvature parameters (a,b,c)

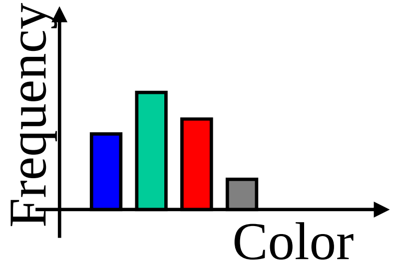
Feature Vectors Associated to Objects



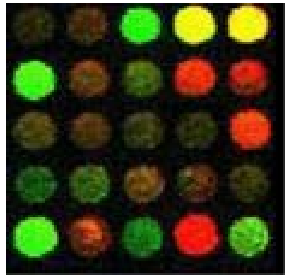
- In a statistical context, we call the features often *variables*.
- The selected features form a *feature vector*
- The feature space is often high-dimensional (in our example 5-D)

Further Examples of Features

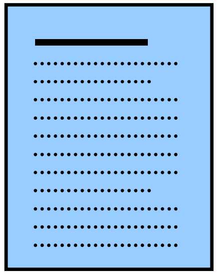
Image Databases:
Color Histograms



Genetic Databases:
Level of Gene Expression



Text-/Document-DBs:
Frequency of terms



Data	25
Mining	15
Feature	12
Object	7
...	

The feature-based approach facilitates a uniform methodology for a great variety of applications

Levels of Measurement

Nominal (Categorical)

Properties:

We can only determine if two values are equal or not. No „better“ and „worse“, no directions.
Features with 2 possible values are called *dichotome*

Examples:

Gender (dichotome)
Eye/Hair Color
Healthy/sick (dichotome)

Ordinal

Properties:

We have a ordering relation (like „better“, „worse“) among the values but not a uniform distance.

Examples:

Quality grade (A/B/C)
Age class (child, teen, adult,senior)
Questionaire answer: (completely agree,…)

Numeric

Properties:

Differences and proportions can be determined. Values can be discrete or continuous.

Examples:

Weight (continuous)
Number of sales (discrete)
Age (contin. or discrete)

Similarity Queries

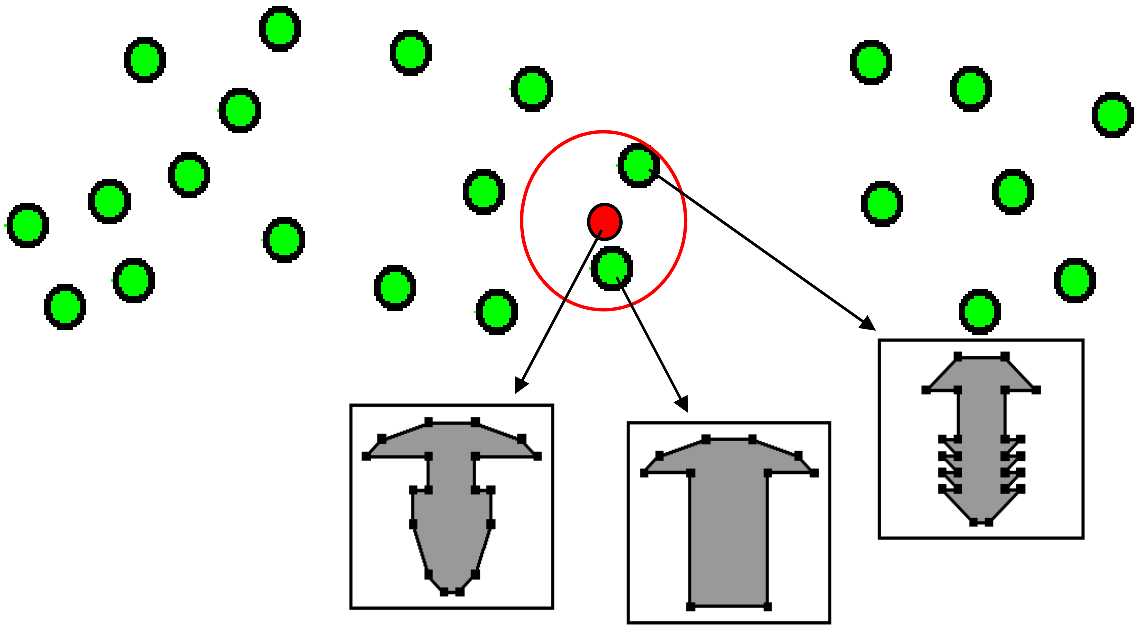
- Specify query-object $q \in$DB and…
  - … search threshold-based (ε) for similar o. – Range-Query

$$RQ(q,\varepsilon) = \{ o \in DB \mid \delta(q,o) \leq \varepsilon \}$$

  - … search for the *k* most similar objects – Nearest Neighbor

$$NN(q,k) \subseteq DB \text{ having at least } k \text{ objects, such that}$$

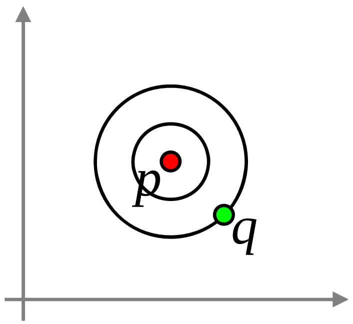
$$\forall o \in NN(q,k),\ p \in DB\text{-}NN(q,k) : \delta(q,o) < \delta(q,p)$$



Similarity of Objects

Euklidean distance (L_2):

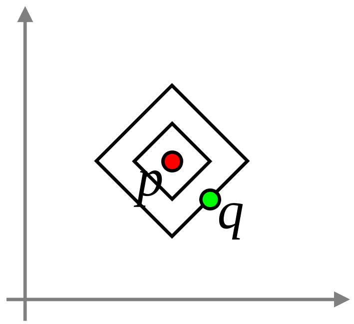
$\delta_2 = ((p_1 - q_1)^2 + (p_2 - q_2)^2 + \ldots)^{1/2}$



Most natural measure of Dissimilarity

Manhattan-Distance (L_1):

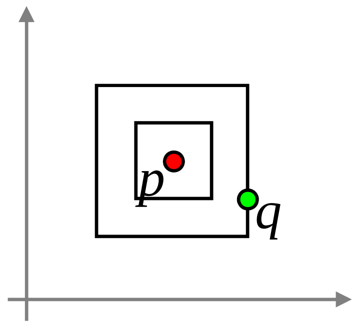
$\delta_1 = |p_1 - q_1| + |p_2 - q_2| + \ldots$



The individual dissimilarities of the features are summed up

Maximum-Distance (L_∞):

$\delta_\infty = \max\{|p_1 - q_1|, |p_2 - q_2|, \ldots\}$



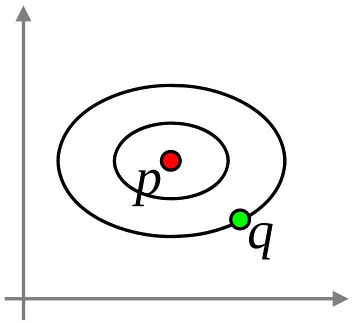
Only the dissmilarity of the least similar feature is taken into account

Generalization L_p-Distance: $\delta_p = (|p_1 - q_1|^p + |p_2 - q_2|^p + \ldots)^{1/p}$

Adaptable Similarity Measures

Weighted Euklidean distance:

$\delta = (w_1(p_1 - q_1)^2 + w_2(p_2 - q_2)^2 + \ldots)^{1/2}$



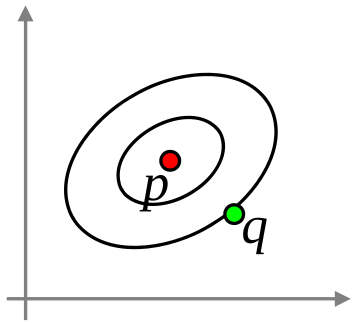
Often the features have (heavily) varying value ranges:

Example: Feature $F_1 \in [0.01 .. 0.05]$
Feature $F_2 \in [3.1 .. 22.2]$

We need a high weight for F_1
(otherwise δ would ignore F_1)

Quadratic form distance:

$\delta = ((p - q)\, M\, (p - q)^T)^{1/2}$



Sometimes we need a common weighting of different features to capture dependencies,
e.g. in color histograms to take color similarities into account

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Some methods do not work with distance measures (where =0 means equality) but with positive similarity measures (=1 means equality)

Data Mining Tasks

Most important data mining tasks based on feature vectors:

Classification
Regression
Clustering
Outlier Detection

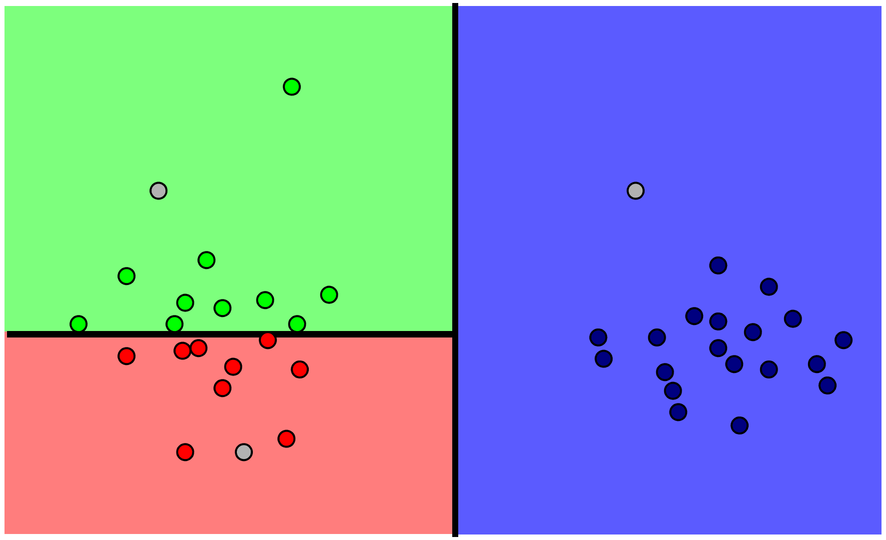
Classification, Regression: Supervised Learning

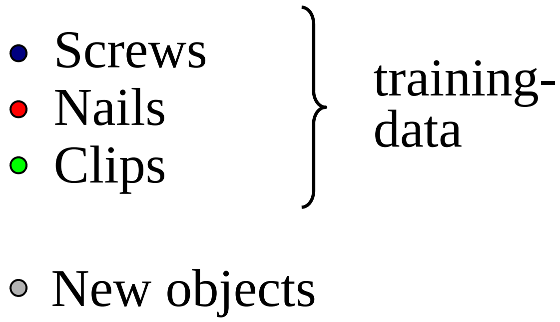
Clustering, Outlier Detection: Unsupervised Learning, Exploratory Analysis

Supervised: Learn rules to predict a previously identified feature
Unsupervised: Learn some regularity/rules

But there is a plethora of methods and tasks not based on feature vectors but directly working on text, sets, graphs etc.

Classification



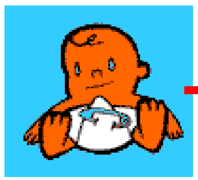


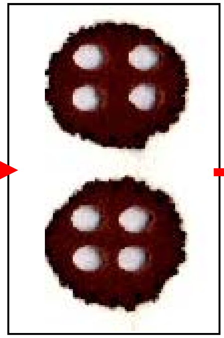
Task:
Learn from previously classified *training data* the *rules*, to predict the class of new objects just based on their properties (features)

The result feature (class variable) is nominal (*categorical*)

Application: Newborn Screening

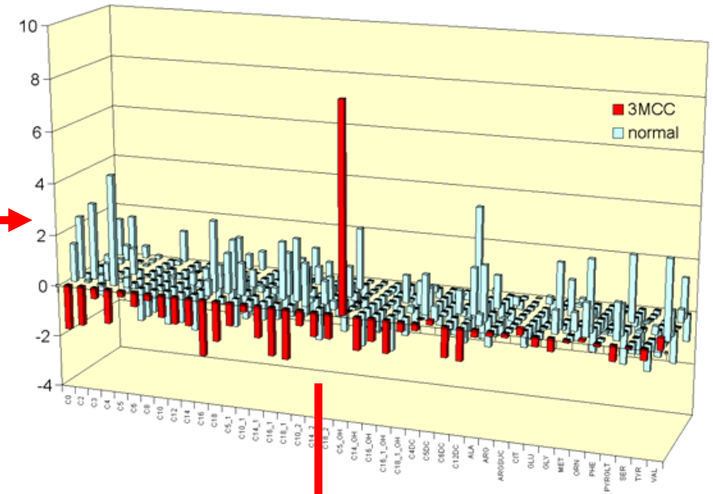
Blood sample of a newborn

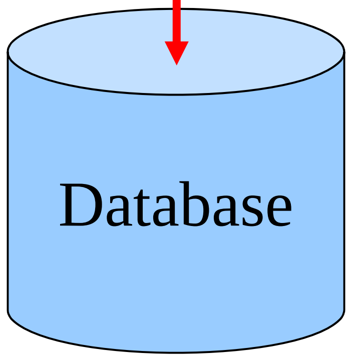




Mass spektrometry

Metabolite spectrum



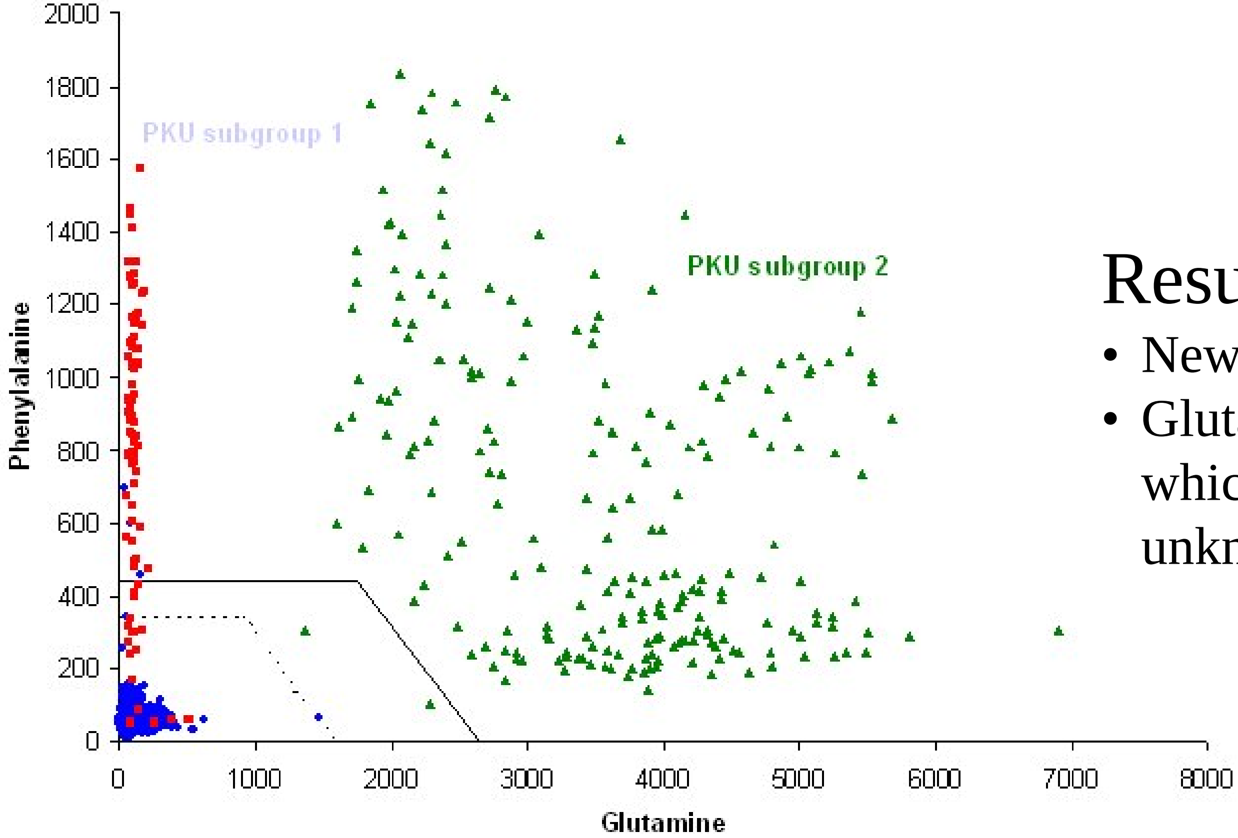


14 analysed amino acids:

alanine	phenylalanine
arginine	pyroglutamate
argininosuccinate	serine
citrulline	tyrosine
glutamate	valine
glycine	leuzine+isoleuzine
methionine	ornitine

[Baumgartner et al., Bioinformatics 20(17), 2004]

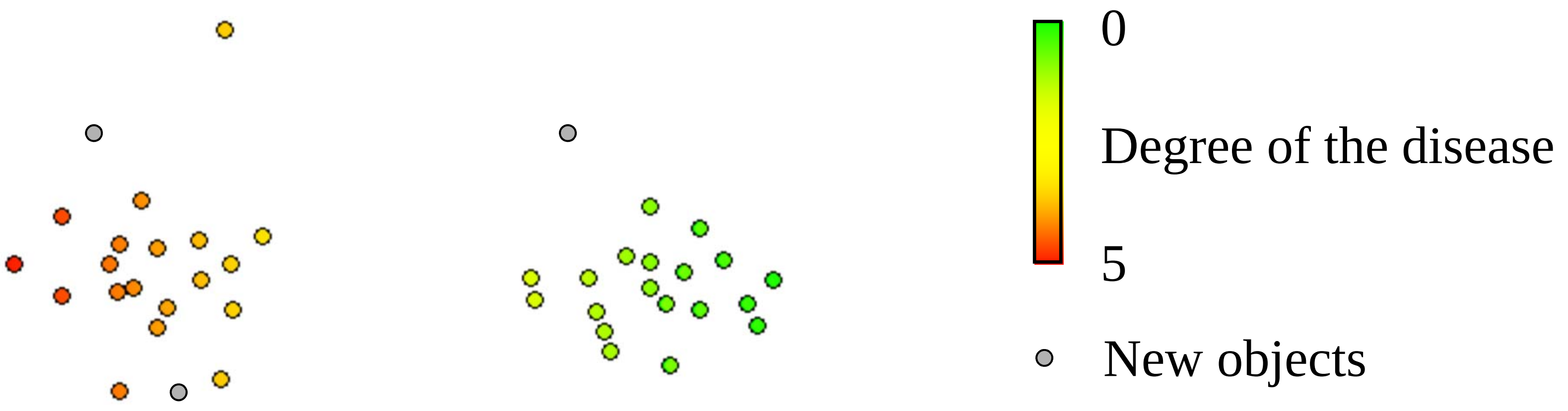
Application: Newborn Screening



Result:

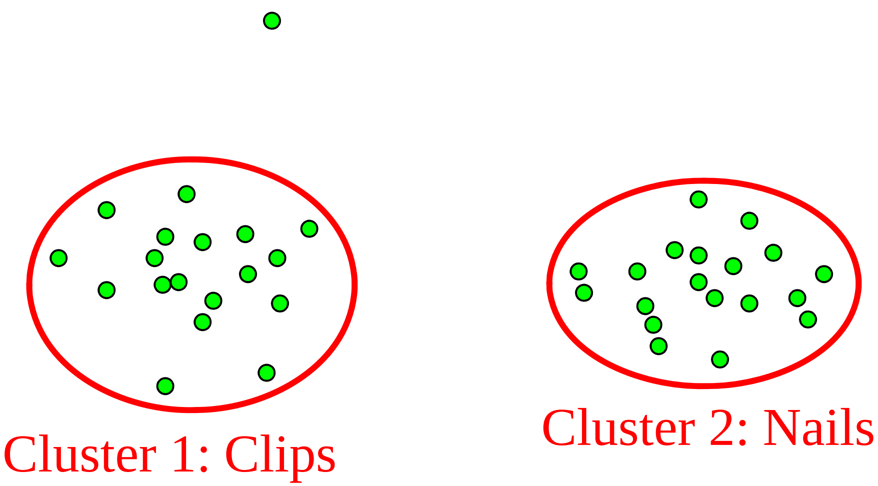
- New diagnostic test
- Glutamine is a marker which was previously unknown

Regression



task:
Similar as classification, but the result feature to be predicted or estimated, ist *numeric*

Clustering



Clustering means: Decompose a set of objects (a set of feature vektors) into subsets (called clusters), such that

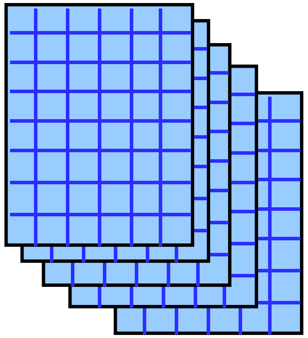
- the similarity of objects of the same cluster is maximized
- the similarity of objects of different clusters is minimized

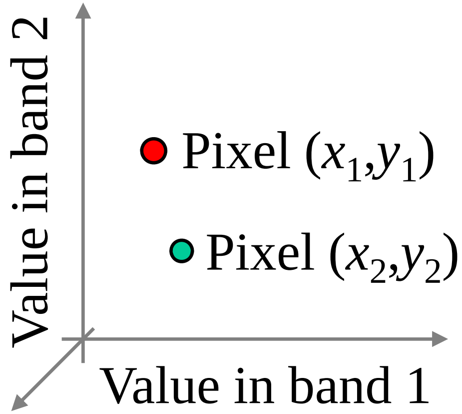
Motivation: Different clusters represent different classes of objects

In contrast to classification: Number and meaning of the classes is unknown.

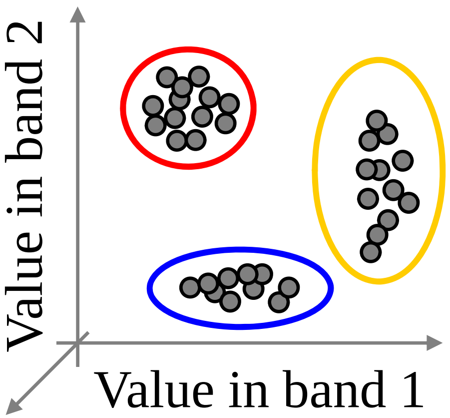
Application: Generation of Thematic Maps

Image of earth surface
in 5 different color spectra



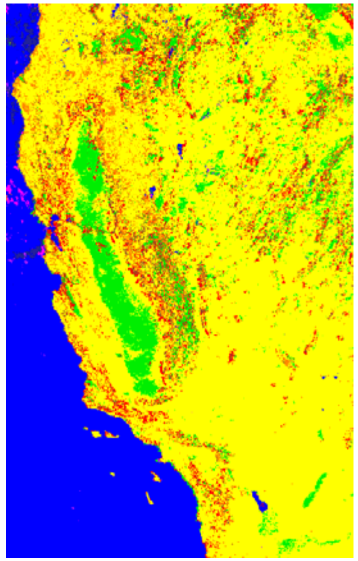


Cluster-Analysis

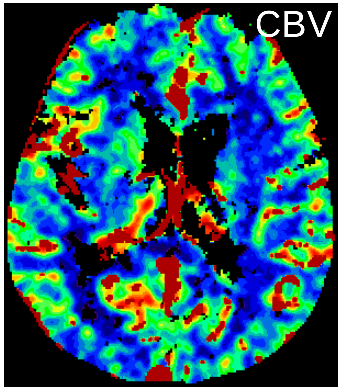


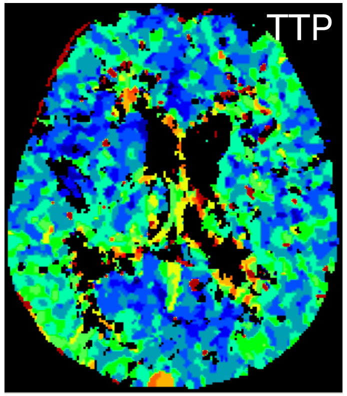
Retransform into
xy-Coordinates

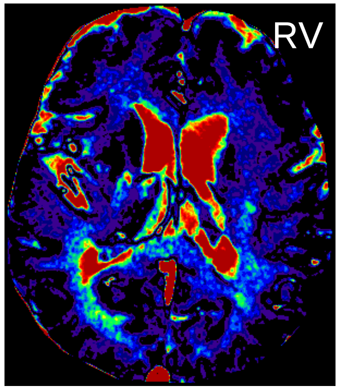
Color coding of
Cluster-membership



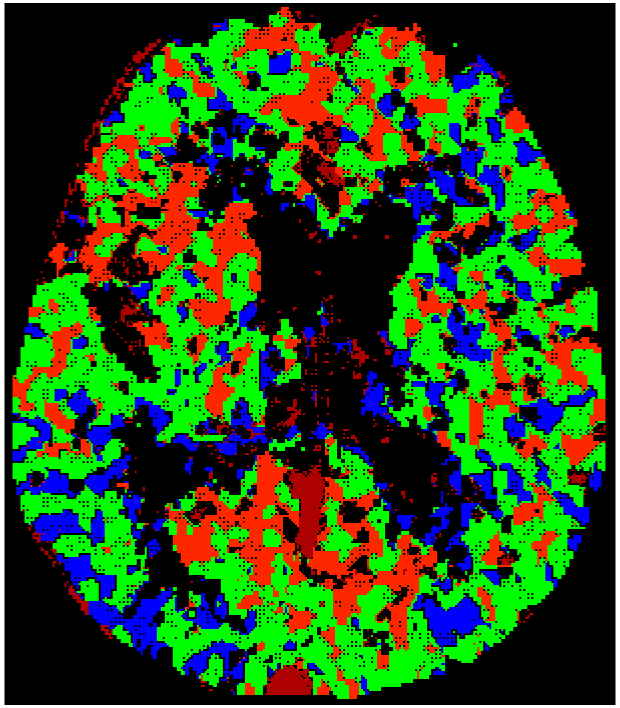
Application: Tissue Classification







- Black: Ventricle + Background
- Blue: Tissue 1
- Green: Tissue 2
- Red: Tissue 3
- Dark red: Big vessels

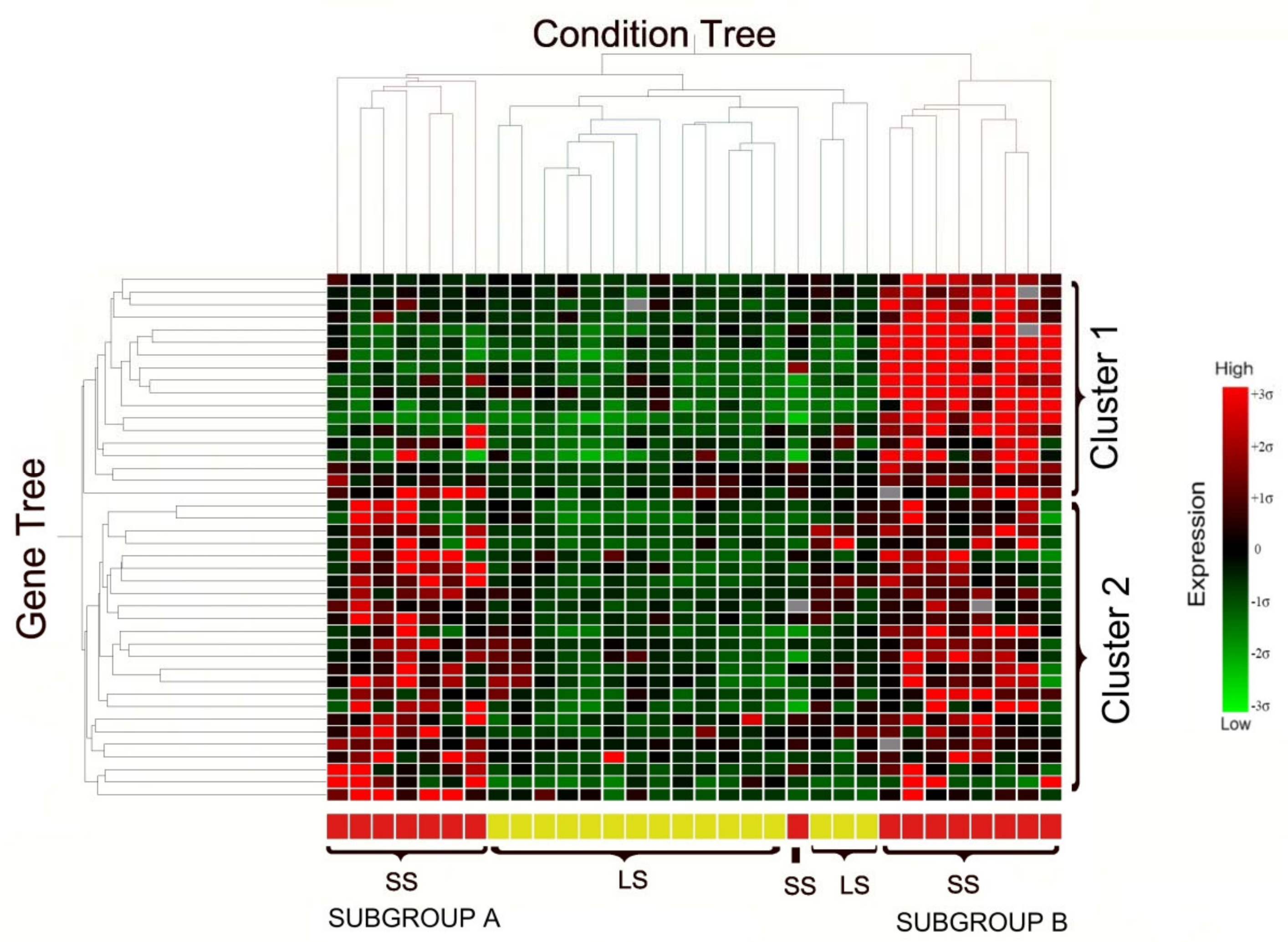


	Blue	Green	Red
TTP (s)	**20.5**	**18.5**	**16.5**
CBV (ml/100g)	**3.0**	**3.1**	**3.6**
CBF (ml/100g/min)	**18**	**21**	**28**
RV	**30**	**23**	**21**

Result: Automatic classification of cerebral tissue possible with dynamic CT.

[Baumgartner et al.: J. Digital Imaging 18(3), 2005]

Application: Gene expression clustering



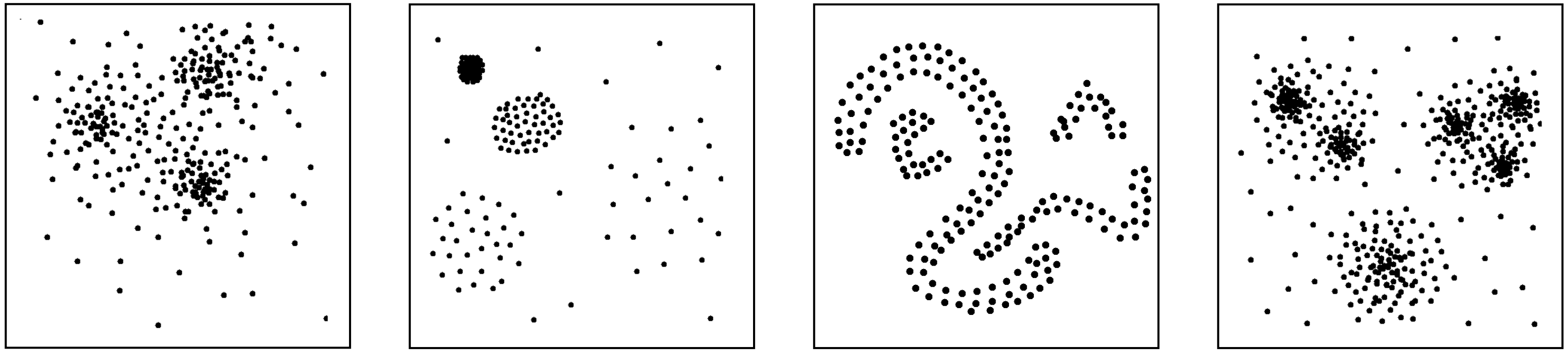
Genes and conditions are **hierarchically** clustered (dendrogram)
Simultaneous row and column clustering is called **co-clustering**

Goals of Clustering

Challenges:

- Clusters of varying size, form, and density
- Hierarchical clusters
- Noise and outliers

=> We need different clustering algorithms



K-Means

- Goal
  - Partitioning into *k* clusters such that a cost function (to measure the quality) is minimized
  - *k* is a parameter of the method (specified by user).

- Locally optimizing method
  - Choose *k* initial cluster representatives
  - Optimize these representatives iteratively
  - Assign each object to its closest or most probable representative
  - Repeat optimization and assignment until no more change (convergence)

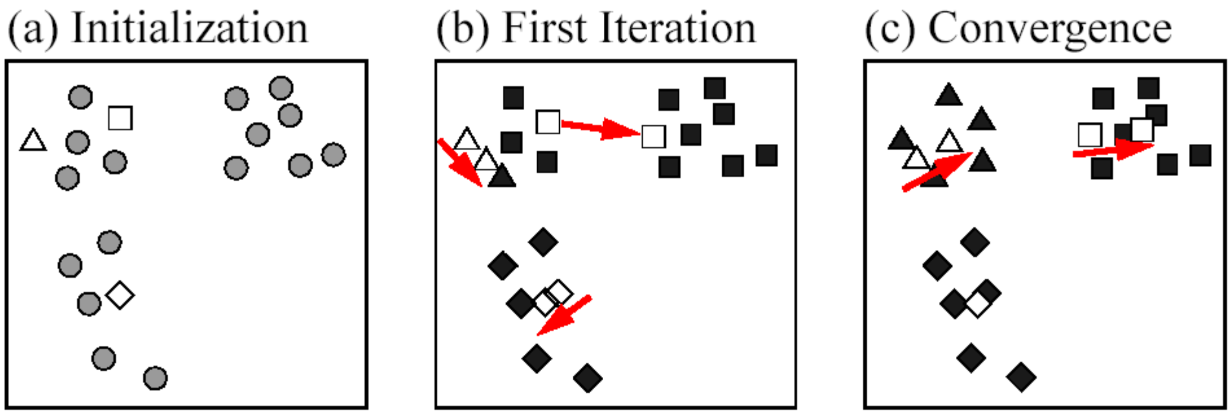
- Types of cluster representants
  - Center (mean, centroid) of each cluster → k-means clustering
  - Most central data object assinged to cluster (*medoid*) → k-medoid clusteing
  - Probability distribution of the cluster → expectation maximization

[Duda, Hart: Pattern Classification and Scene Analysis, 1973]

K-Means

Idea of the algorithm

- Algorithmus starts e.g. with randomly chosen objects as initial cluster representatives (many other initialization methods have been proposed)
- The algorithm is composed from two alternating steps:
  - Assignment of each point to ist closest representative point
  - Recomputation of the cluster representative (center of its objects)
- Repeat the alternating steps until no more change (convergence)



K-Means

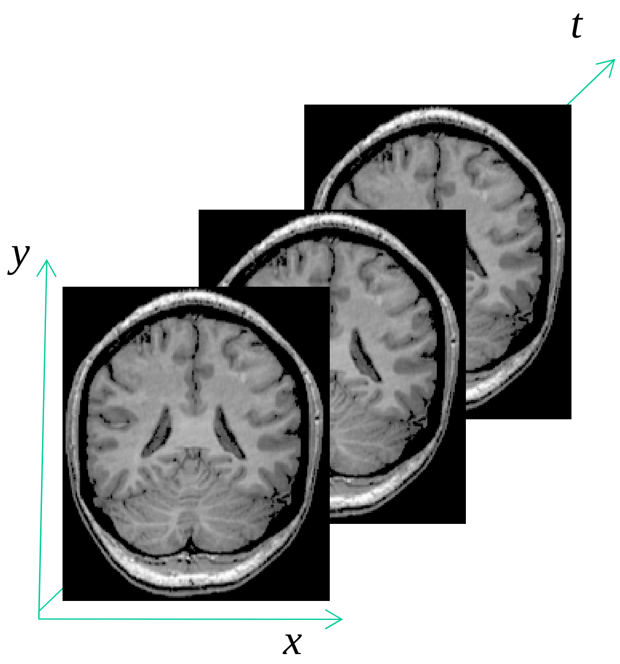
Properties of the algorithm

- Fast convergence to a *local* minimum of the objective function (Variance of the clusters, averaged over all clusters and dimensions)

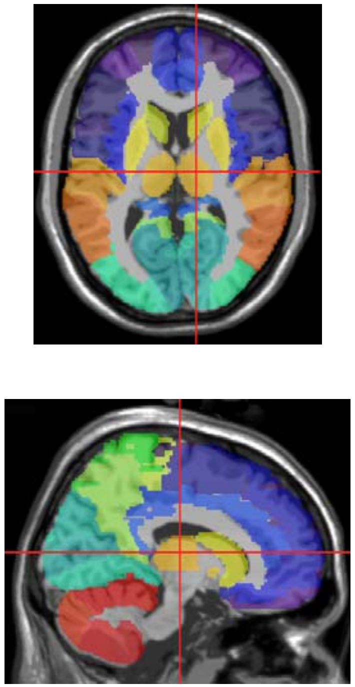
$$J = \sum_{j=1}^{k} \sum_{i=1}^{n} \left\| x_i^{(j)} - c_j \right\|^2$$

- It is easy to see that
  - Assignment of points to clusters minimizes the objective function.
  - Re-determination of cluster centers minimizes the objective function.
- Thus the objective function is monotonic and bounded.
- Typically a small number of iterations (3-50) needed.
- To find the *global* optimum is more difficult (NP-hard in general)
  - Typical heuristic: Multiple (e.g. 10) runs with different initialisations of the starting points

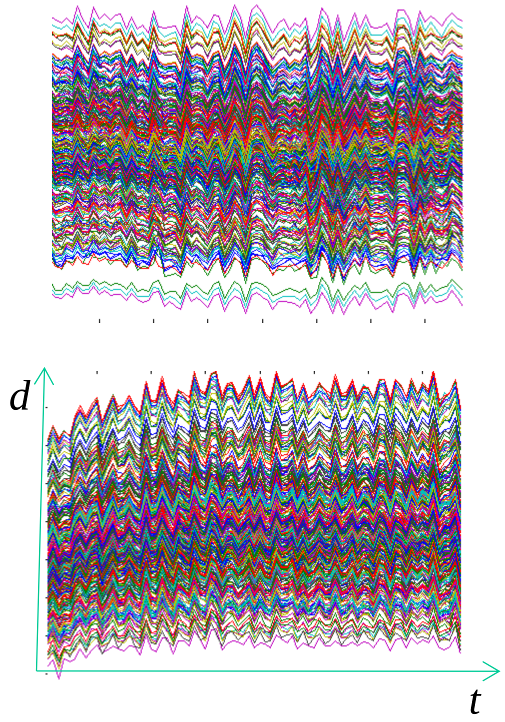
Mining Interaction Patterns of Brain Regions



fMRI data:
Time Series of 3d volume images of the brain.



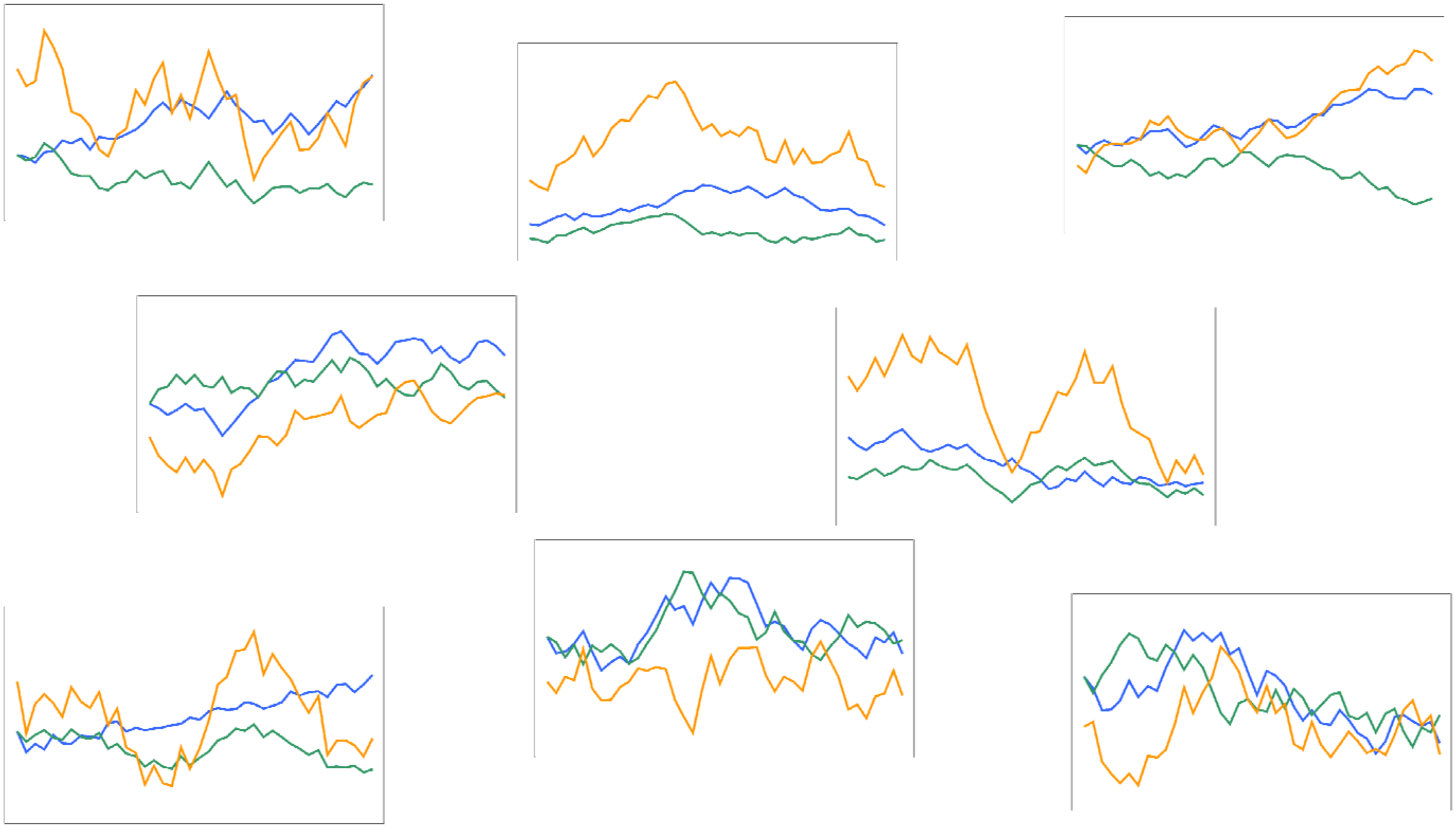
Parcellation into 90 anatomical regions.



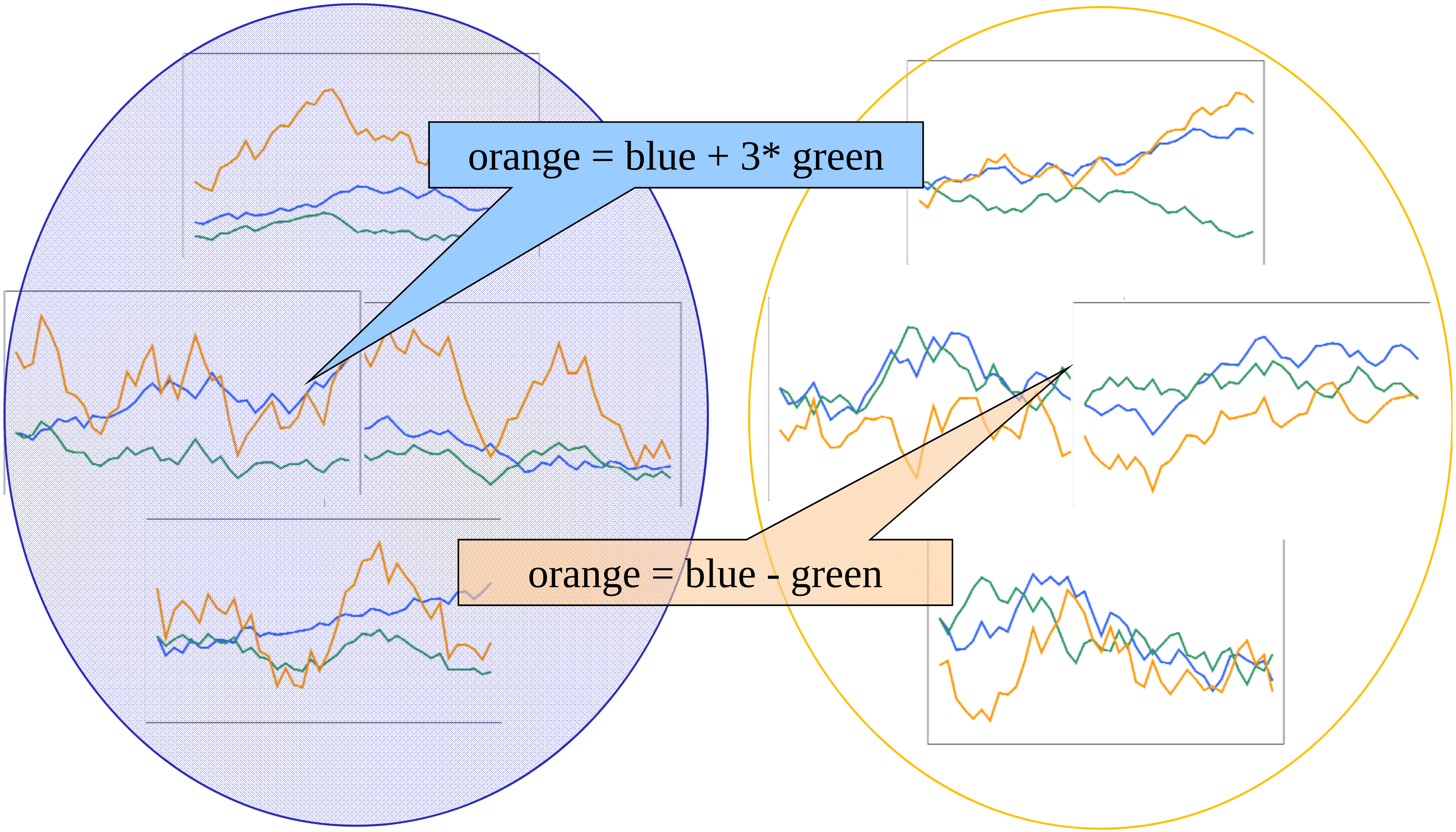
Each person is represented by a multivariate times series with *d* = 90 dimensions.

[Plant, Wohlschläger, Zherdin: ICDM 2009]

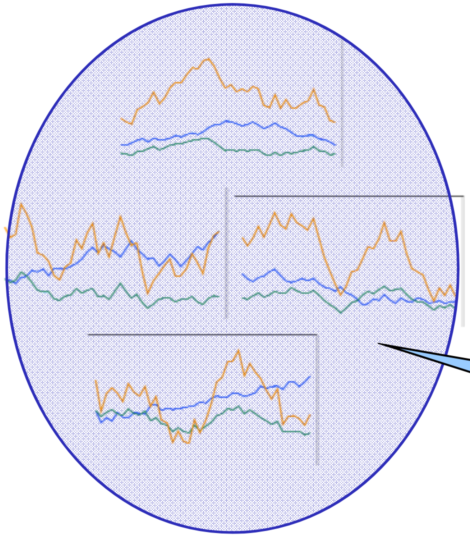
Clustering Multivariate Time Series



…by Interaction Patterns



Interaction-based Cluster Notion



Cluster:

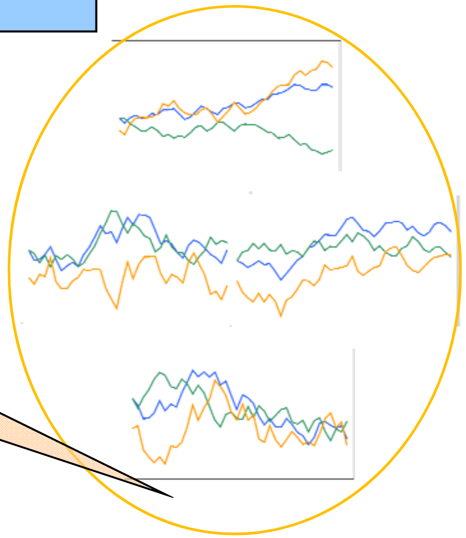
- set of *linear models* representing the dependency of each single Y dimension w.r.t. other dimensions X

$$Y = X\beta + \varepsilon$$

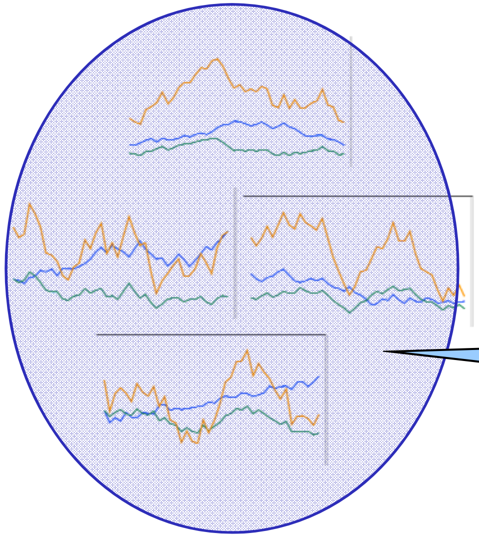
orange = blue + 3* green + ε
blue = …
green = …

- *set of objects.*

orange = blue – green + ε
blue = …
green = …



Model Finding

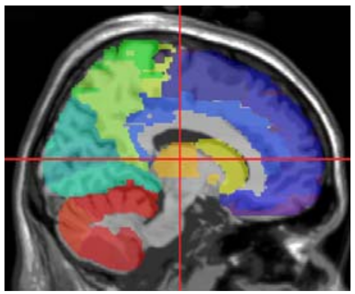


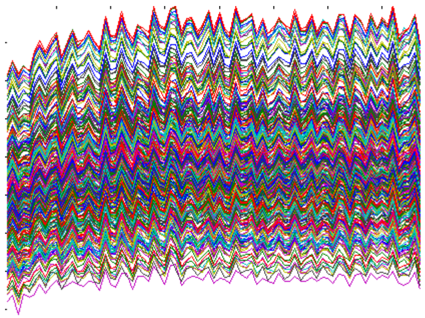
Set of *linear models* representing the dependency of each single Y dimension w.r.t**. other dimensions X**

$$Y1 = X1 * \beta + \varepsilon$$
$$Y2 = X2 * \beta + \varepsilon$$
$$\ldots$$
$$YD = XD * \beta + \varepsilon$$

Can be straightforward solved by multidimensional linear regression

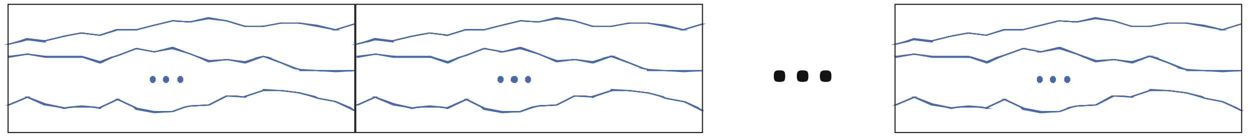
But which dimensions X should be applied?





Usually not all *d* dimensions…

Greedy Stepwise Regression Controlled by BIC



First concatenate all objects of the cluster,

then greedily add and remove dimensions
evaluating intermediate results with Bayesian Information Criterion (BIC).

$$Y = X\beta + \varepsilon \text{ and } \beta = (X^T X)^{-1}(X^T Y)$$

$$BIC(M) = -2L_n(\hat{\beta}, \hat{\sigma}^2_{ML}) + \log(n)(\dim \beta + 1)$$

$$L_n(\hat{\beta}, \hat{\sigma}^2_{ML}) = -\frac{n}{2} - \frac{n}{2}\log \hat{\sigma}^2_{ML} - \frac{n}{2}\log(2\pi)$$

$$\hat{\sigma}^2_{ML} = \frac{1}{n} \| Y - X\beta \|^2$$

Algorithm Interaction K-means (IKM)

1) Initialization: Random partitioning into K equally sized clusters
2) Iterate the following steps until convergence:

***Assignment*:** Assign each object to that cluster to which it has the smallest sum of errors over all *d* dimensions

Update: Apply greedy-stepwise regression with BIC to all clusters.

Major differences to standard K-means:

- similarity measure is the sum of errors of an object w.r.t. a set of models

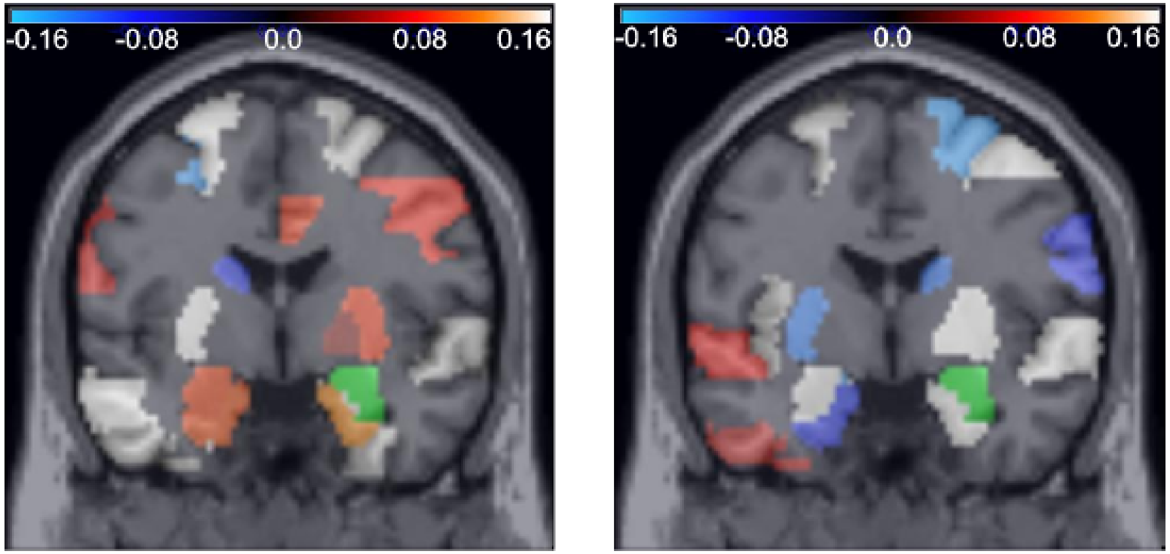
- Cluster representative is not an object but *a set of models describing characteristic interaction patterns* shared by the objects within the cluster.

Inherited from K-means: Efficiency due to fast convergene;
Further improvement by aggregative pre-computing;

Results: Interaction patterns of brain regions

- resulting from clustering fMRI data with IKM.
- study on Somatoform Pain Disorder (pain without any clinical cause).
- Task fMRI: while in scanner the persons have been exposed to painful stimuli.

control *somatoform*



Right Amygdala (green) is interacting with different regions in patients and controls:
- controls: sensory areas (temporal, auditory)
- patients: frontal control areas.

Only useful for this special fMRI application?

- also effective on synthethic and publicly available benchmark data from various domains.

- in comparison to standard K-means (Naive) and the state-of-the-art approach: Statistical Features Clustering (SF) (Wang et al., ICDM 2007)

Data Set	Method	RI	IC
DS1 Synthetic K=6, $n = 600$, $d = 13$, $m = 3333$	IKM SF Naive	**0.99** 0.49 0.72	**0.09** 1.48 2.38
DS2 fMRI K=2, $n = 26$, $d = 90$, $m = 216$ or 325	IKM SF Naive	**0.56** 0.48 0.49	**0.89** 1 0.98
DS3 EEG K=2, $n = 20$, $d = 64$, $m = 256$	IKM SF Naive	**1** 0.61 0.49	**0** 0.69 0.95
DS4 CAD K=10, $n = 100$, $d = 25$, $m = 70$	IKM SF Naive	0.91 0.92 **0.98**	0.91 0.95 **0.2**
DS5 Japanese vowels K=9, $n = 640$, $d = 12$, $m = 7$-29	IKM SF Naive	**0.88** 0.79 0.83	**1.21** 2.36 2.04

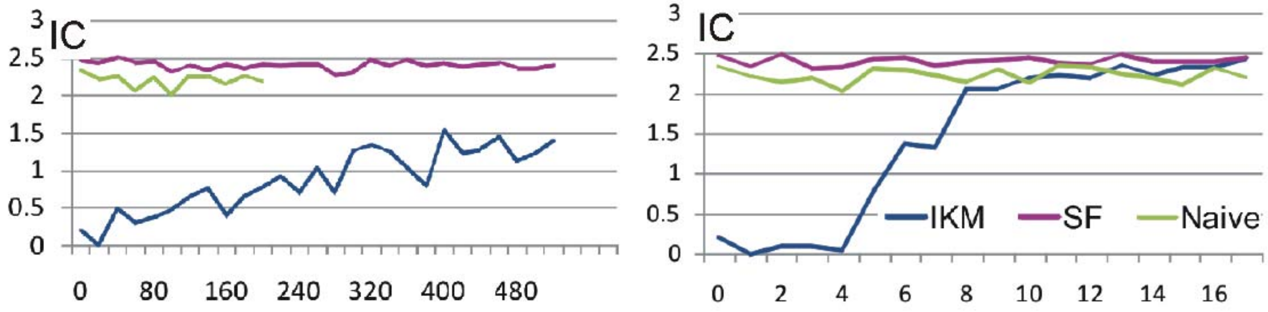
EEG data (UCI)

motion streams

language processing (UCI)

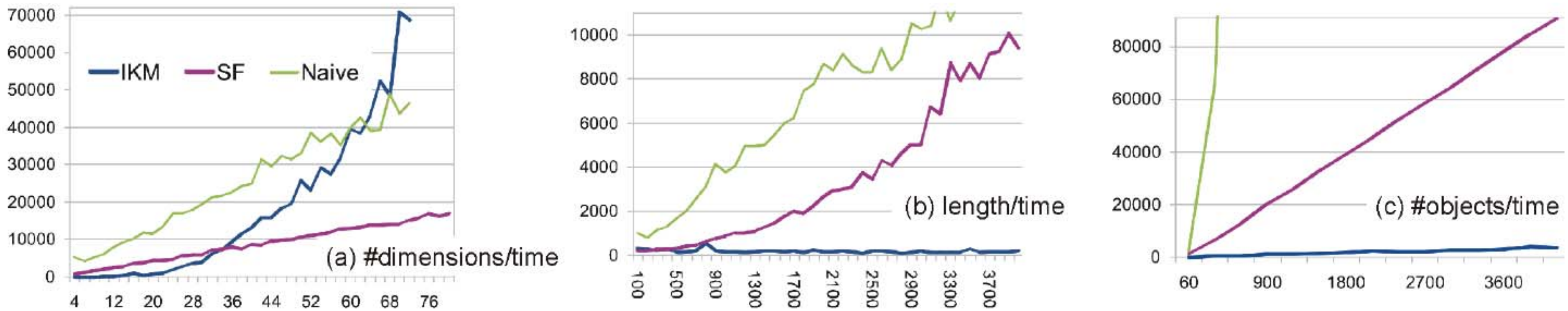
Further Benefits of IKM

- **Robust against noise objects and noise dimensions,**



(a) Noise-Obejcts (b) Noise-Dimensions

- **Scalable,**



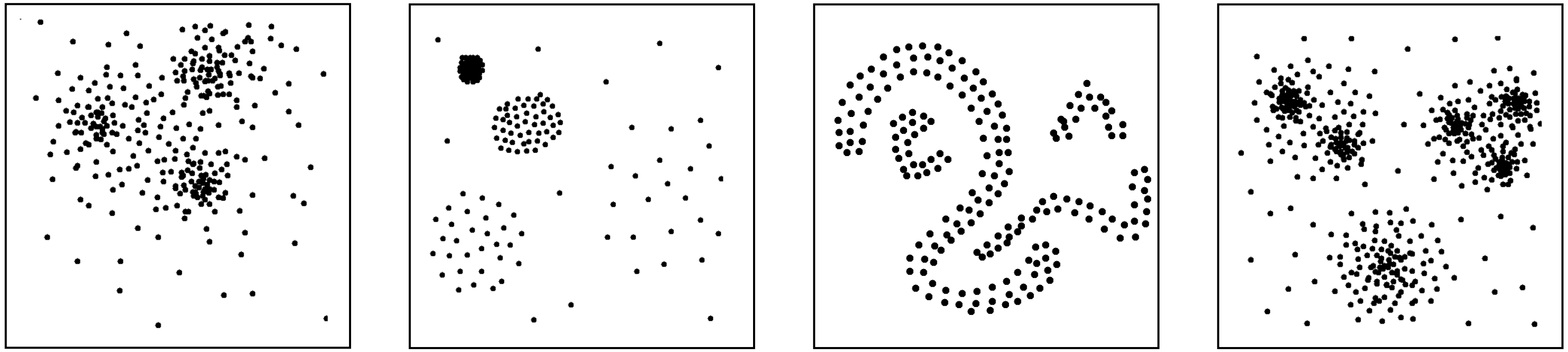
- and does not require all objects having time series of equal length.

Goals of Clustering

Challenges:

- Clusters of varying size, form, and density
- Hierarchical clusters
- Noise and outliers

➔ We need different clustering algorithms



(1) (2) (3) (4)

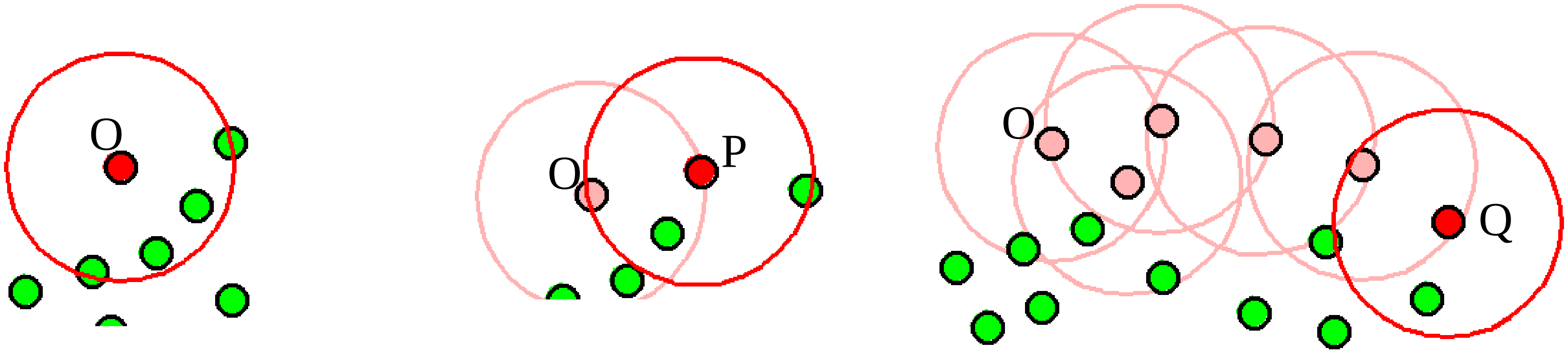
K-Means can handle compact, spherical clusters like in (1)

For clusters with arbitrary shape like (3) we need a different clustering notion:

- Density-Based Clustering

Density-based Clustering with DBSCAN

Idea: Clusters are areas of high object density which are separated by areas of lower Object density.



O is a **core object** if
There are least MinPts objects
within it's ε-range.

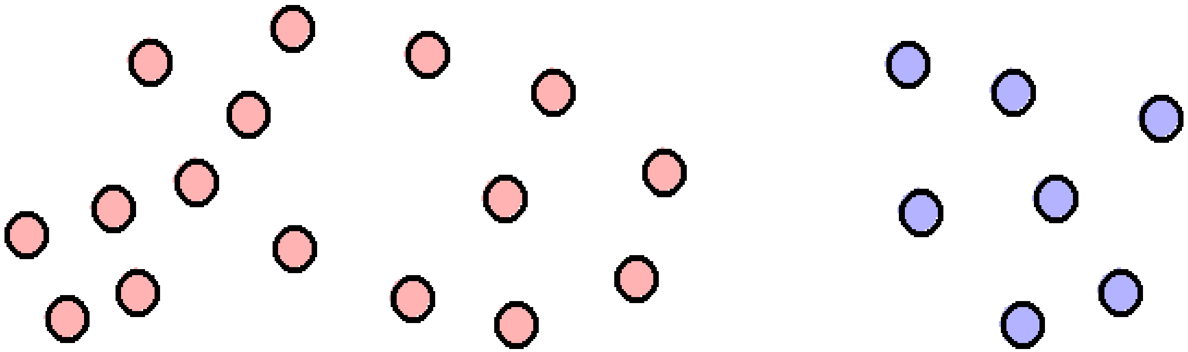
P is **directly density-reachable**
from O if O is a core object
and P is within the ε-range of O.

O and Q are **density-connected** if
they are connected by a chain of
density-reachable objects.

A **density-based cluster** is a maximal set of density-connected objects.

[Ester et al. KDD 1996]

DBSCAN - Example



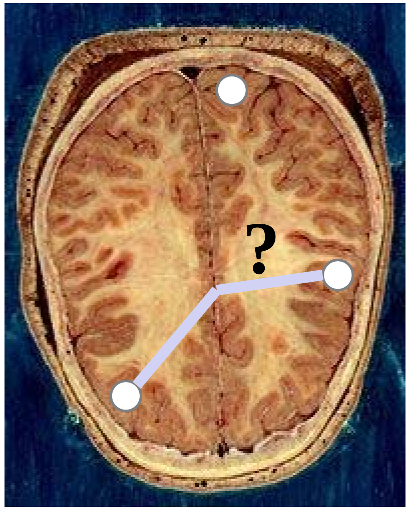
Start cluster expansion with an arbitrary core object;
add objects within ε-range into seedList;
While the seed list is not empty:

Remove top element; set its cluster Id;

If it is a core object: add objects within ε-range to seed list as well.

Understanding the connectome of the brain

Basic anatomy of the brain:



Grey Matter: neuronal cell bodies
White Matter: myelinated axons
The brain is a highly efficient network!

But what are the nodes or functional units ?

And what are the edges or major highways?

Why is this important to know?
- surgery planning (epilepsy, tumor),
- understanding brain development during adolescence and normal aging,
- understanding the onset and progression of neurodegenerative diseases like Alzheimer.

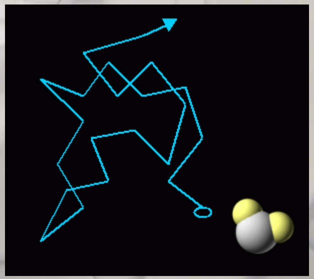
[Shao et al., ICDM Workshop 2010]

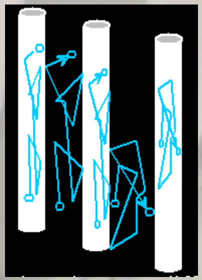
Visualizing the White Matter by diffusion tensor imaging (DTI)

Basic Principle

- movement of water molecules is restricted by white matter;
- in magnetic field moving molecules emit radiofrequency signals;

- DTI measures strength and direction of movement with 2 magnetic pulses coming from a specific direction called gradient:
  the first pulse labels the molecules,
  the second pulse reads out the displacement in a voxel in the gradient direction.

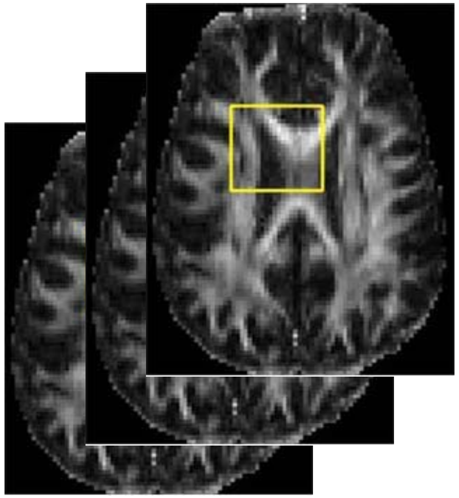




- Different gradient images need to
  be combined to capture the 3-d diffusion, 55 on our experimental data

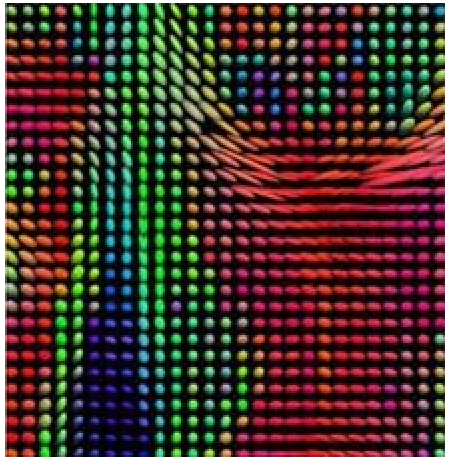
Preprocessing: Fiber Tracking

(1) Combination: Motion correction, co-registration



55 gradient images

(1)



Diffusion tensor field
256x256x70 -> 4,578,520 voxels

(2)

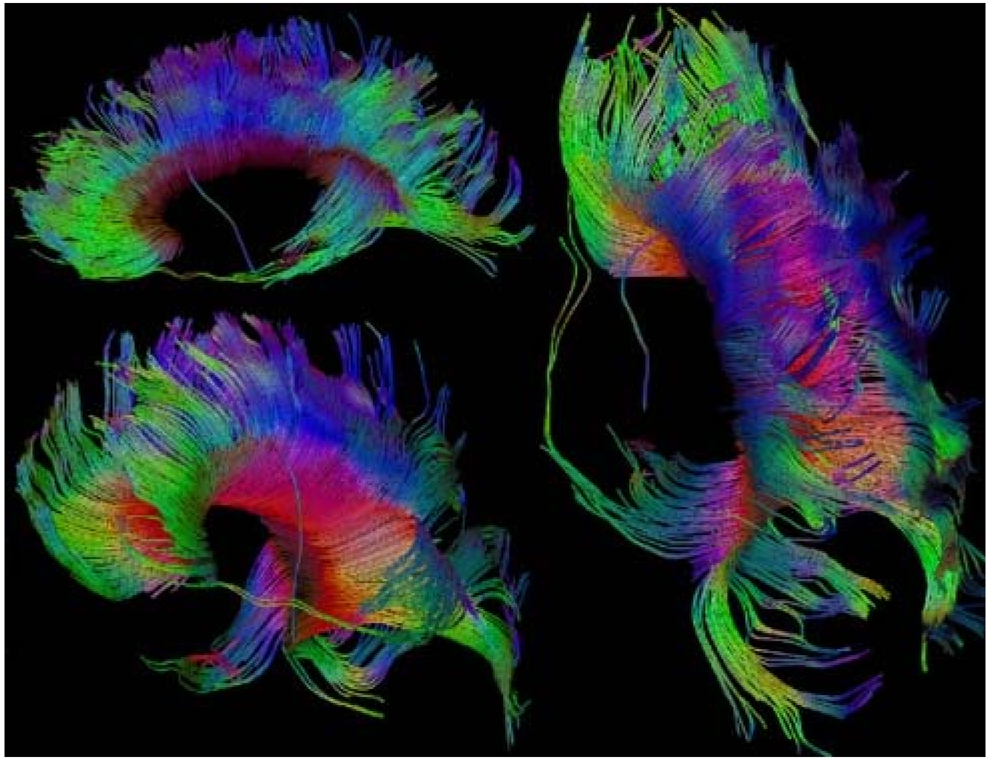
Thousands of fibers

(2) Fiber Tracking
Runge Kutta Method (4th order):

- requires pre-defined seed and end region
- a fiber is modeled as a 3-d discrete curve which is drawn step by step
- select the next voxel by solving an ordinary differential equation involving the leading Eigenvector of the ellipsoid, the start and the end point

Still too much information!

What are the major highways ?



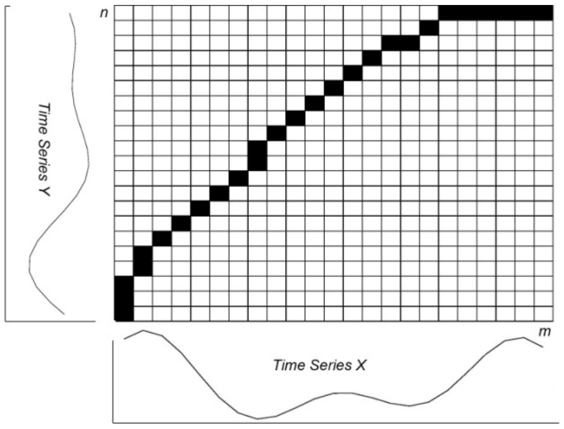
More than 1,000 fibers only for the Corpus Callosum

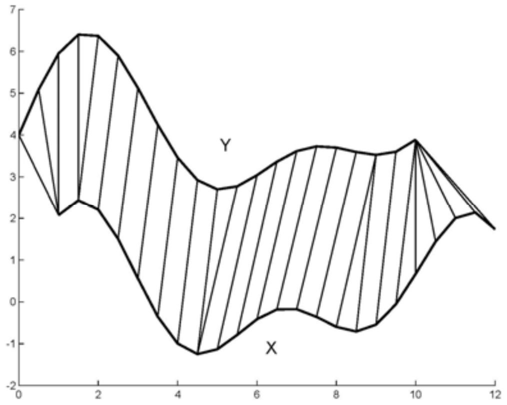
Hundreds of thousands fibers in the brain

-> Fiber Clustering – suitable to deal with noise!
-> We need an effective and efficient similarity measure!

Evaluating similarity by 3-d fiber warping

Strength of DTW:
Optimal local alignment of timeseries to capture local similarity

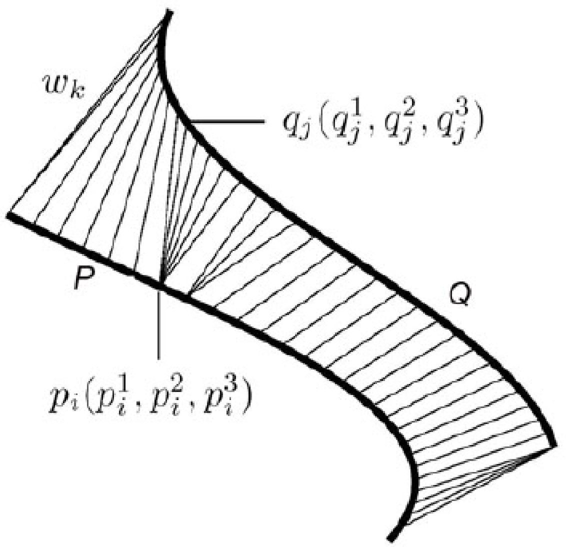




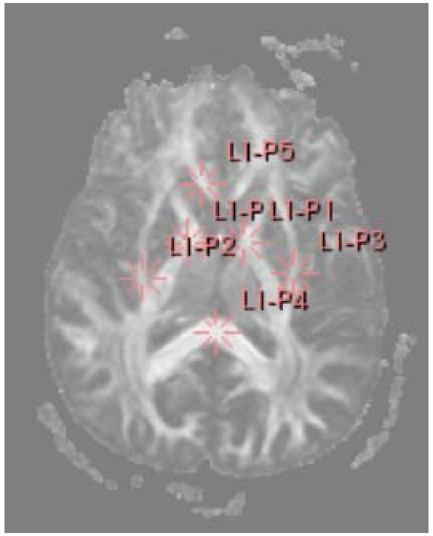
Extending DTW to 3 dimensions:

$$d(p_i, q_j) = |p_i^1 - q_j^1| + |p_i^2 - q_j^2| + |p_i^3 - q_j^3|$$

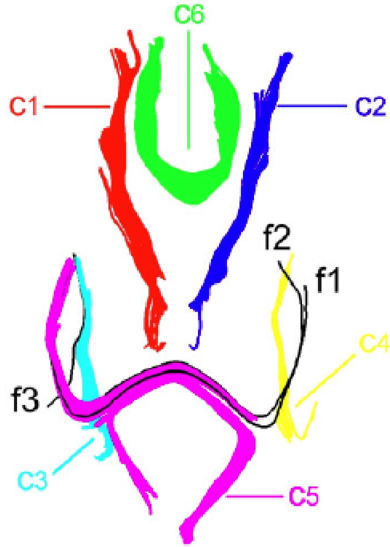
- Optimal Warping Path is determined using Quadratic programming as for DTW
- Avoiding that the fiber length overly dominates the similarity: Averaging all point-to point distances along the optimal warping path.



Experiments – Similarity Measure



6 seed regions
For fiber tracking
in the internal and
external Capsules
and the Corpus Callosum



Fibers grouped by
medical experts into the
corresponding 6 bundles
and 3 outlying
fibers

DTW

perfect

MPC

Outliers
Assigned to cluster

(mean of closest pairwise distances)

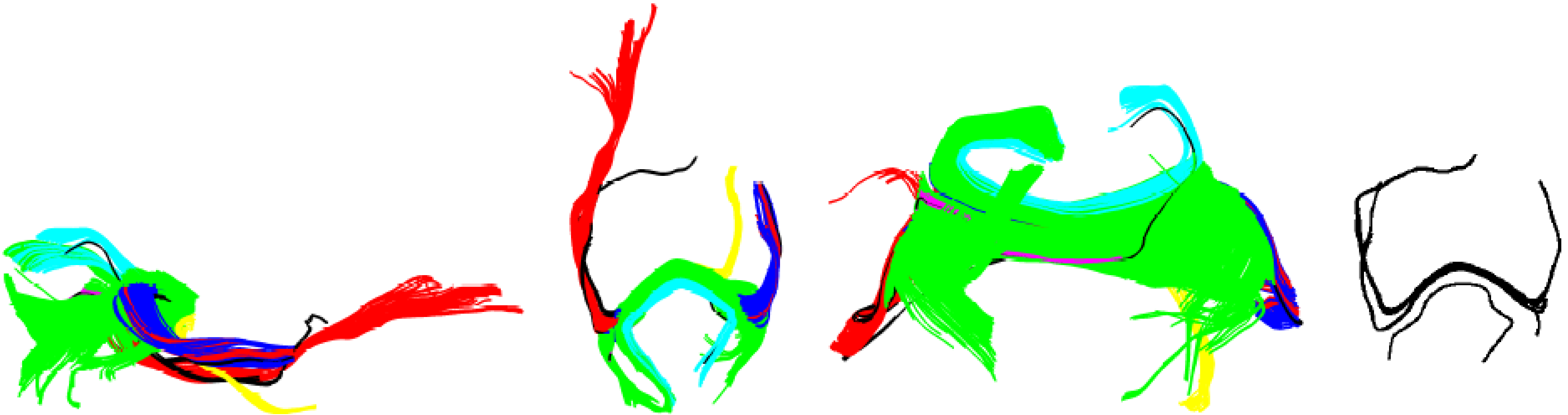
Haussdorff

10 clusters

(maximum of longest pair-wise distances)

Results

Effective detection of clusters of different size and separation of noise → DBSCAN is good!



(a) Sagittal (b) Axial (c) Coronal (d) Axial (Noise)

Data Set 2: 973 fibers

What have we learned?

- Data Mining (Knowledge Discovery in Databases, KDD) is a central technology to cope with Big Data.
- Feature vectors are the most common objects used in data mining
- We distinguish between two philosophies
  - Supervised (attribute to be predicted is known)
  - Unsupervised (exploratory data analysis)
- Clustering is an unsupervised technique to group objects
  - Maximize intra-cluster similarity
  - Minimize between-cluster similarity
- There exists a large number of approaches with different properties:
  - Partitioning clustering like K-Means (spherical clusters)
  - Density-based clustering like DBSCAN (arbitrary shapes)