Data Mining Tasks

- Classification
- Prediction
- Clustering
- Dependency Modelling
- Summarization
- Change and Deviation Detection
- Visualization

Prediction

- prediction of a (future) category based on observed data → classification
- prediction of a (future) numerical value y based on observed data $\vec{x}$
  - y: response output, dependent variable
  - $\vec{x}$: input, regressors, explanatory variables, independent variables
- applications
  - the output is expensive to measure, the input not
  - the value of the inputs is known before the value of the output and a prediction is required
  - simulation of system behaviour by controlling the inputs
  - detecting causal links between the inputs and the output

Regression

- most common form: linear regression
  - assuming a linar function

$$y = f(\vec{x}) = a_0 + \sum_{i=1}^{n} a_i \cdot x_i$$

  - inserting all m training samples → m new equations

$$y_i = \epsilon_j + a_{0j} + \sum_{i=1}^{n} a_i \cdot x_{ij}$$

$\epsilon_j (j = 1 \ldots m)$: regression error for each given sample

  - modify the linear coefficients a_i to minimize the sum of error squares $e = \sum_{i=1}^{n} \epsilon_i^2$

Regression

- special case: single predictor variable

$$y = f(x) = a_0 + a_1 \cdot x$$

$$e = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - y_i')^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$$

- minimizing for a_0 and a_1

$$\frac{\delta e}{\delta a_0} = -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) = 0$$

$$\frac{\delta e}{\delta a_1} = -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) \cdot x_i = 0$$

Regression

- minimizing (cont.)

$$n a_0 + a_1 \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

$$a_0 \sum_{i=1}^{n} x_i + a_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

$$a_0 = \mu_y - a_1 \mu_x$$

$$a_1 = \frac{\sum_{i=1}^{n} (x_i - \mu_x) \cdot (y_i - \mu_y)}{\sum_{i=1}^{n} (x_i - \mu_x)^2}$$

Regression

- multiple regression (multiple predictor variables)

$$y = a_0 + \vec{a}\,\vec{x}$$

$$e = (\vec{y} - a_0 \vec{a} \cdot X)^T \cdot (\vec{y} - a_0 \vec{a} \cdot X)$$

X: Matrix of all data vectors $\vec{x_j}$ from the training set

$$\vec{a} = (X^T \cdot X)^{-1} (X^T \cdot \vec{y})$$

  - solution of equation set requires exponential effort
  - not feasible for realistic training sets

Regression

- identifying the relevant variables
  - selectively add to or delete variables from an initial set
  - testing for a linear relationship: correlation

$$r = \frac{\sum_{i=1}^{n} (x_i - \mu_x) \cdot (y_i - \mu_y)}{\sqrt{\sum_{i=1}^{n} (x_i - \mu_x) \cdot \sum_{i=1}^{n} (y_i - \mu_y)}}$$

Regression

- non-linear relationships
  - transform to a linear equation

polynomial	$y = ax^2 + bx + c$	$x^* = x^2$
exponential	$y = ae^{bx}$	$y^* = \ln y$
power	$y = ax^b$	$y^* = \log y, x^* = \log x$
reciprocal	$y = a + b\frac{1}{x}$	$x^* = \frac{1}{x}$
hyperbolic	$y = \frac{x}{a+bx}$	$y^* = \frac{1}{y}, x^* = \frac{1}{x}$

  - use neural networks to approximate a nonlinear function → low perspicuity

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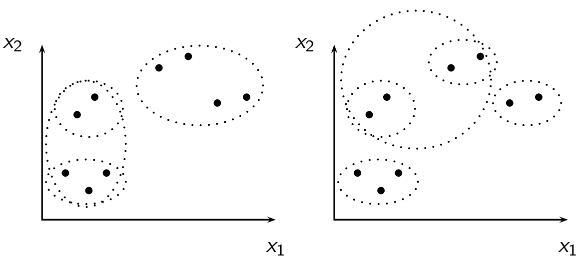
Clustering

- grouping of data points according to their inherent structure
  - based on a similarity measure
  - learning without teacher
- many clustering approaches
  - hierarchical clustering
  - partitioning clustering
  - incremental clustering
  - clustering with neural networks

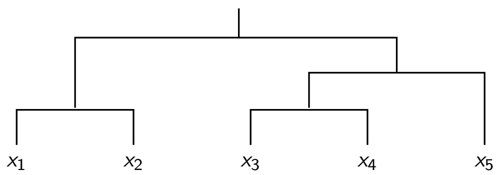
Clustering

- computing the optimal clustering is computationally infeasible
  $\longrightarrow$ greedy, sub-optimal approaches
- different clustering algorithms might lead to different clustering results



Hierarchical Clustering

- agglomerative hierarchical clustering
- successively merging data sets
- result can be displayed as a dendrogram



Hierarchical Clustering

- algorithm
  - initially each cluster consists of a single data point
  - determine all inter-cluster distances
  - merge the least distant clusters into a new one
  - continue until all clusters have been merged

Distance Measures

- distance measure for clusters
  - single link: minimum of distances between all pairs of data points
  - complete link: e.g. mean of distances between all pairs of data points
- local clustering criterion for data points: minimal mutual neighbor distance (MND)
  - distance depends also on the local context of a data point

$$d_{MND}(\vec{x_i}, \vec{x_j}) = r(\vec{x_i}, \vec{x_j}) + r(\vec{x_j}, \vec{x_i})$$

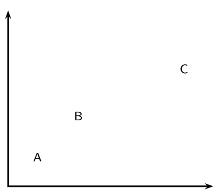
$r(\vec{x_i}, \vec{x_j})$: rank of x_j according to distance from x_i

Partitioning Clustering

- mutual neighbor distance (MND)

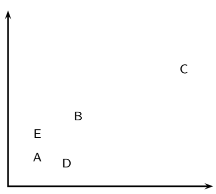
$$\begin{aligned} d_{MND}(A,B) &= r(A,B) + r(B,A) \\ &= 1 + 1 = 2 \end{aligned}$$

$$\begin{aligned} d_{MND}(B,C) &= r(B,C) + r(C,B) \\ &= 2 + 1 = 3 \end{aligned}$$



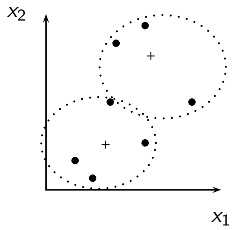
$$\begin{aligned} d_{MND}(A,B) &= r(A,B) + r(B,A) \\ &= 3 + 3 = 6 \end{aligned}$$

$$\begin{aligned} d_{MND}(B,C) &= r(B,C) + r(C,B) \\ &= 4 + 1 = 5 \end{aligned}$$



Partitioning Clustering

- number of resulting clusters is given in advance
- each cluster is represented by a centroid



Partitioning Clustering

- global clustering criterion: minimizing the mean square error
  - mean vector as centroid

$$\vec{c_k} = \frac{1}{n_k} \sum_{i=1}^{n_k} \vec{x_{ik}}$$

  - error for one cluster (within-cluster variation)

$$e_k^2 = \sum_{i=1}^{n_k} (\vec{x_{ik}} - \vec{c_k})^2$$

  - global error

$$e = \sum_{k=1}^{K} e_k^2$$

Partitioning Clustering

- algorithm for k-means partitioning clustering
  - select a randomly chosen initial partitioning with k clusters
  - compute the centroids
  - assign each sample to the nearest centroid
  - compute new centroids
  - continue until the clustering stabilizes (or another termination criterion based on the global error is met)

Incremental Clustering

- huge data sets cannot be clustered in a single step
  - divide-and-conquer: cluster subsets and merge the results
  - incremental clustering: data points are loaded successively and the cluster representation is updated accordingly

Incremental Clustering

- algorithm
  - assign the first data point to the first cluster
  - consider the next data point
    - assign it to an already existing cluster, or
    - create a new cluster
  - recompute the cluster description for that cluster
  - continue until all data points are clustered

Incremental Clustering

- cluster description
  - centroid
  - number of data points in the cluster
  - "radius" of the cluster (based on the mean-squared distance to the centroid)
- problems
  - result depends on the order in which data points are processed → iterative incremental clustering
    - use the centroids of the previous iteration for partitioning in the next one

Clustering with Neural Networks

- competitive learning
  - single layer network
  - each output neuron corresponds to a cluster
  - the neurons are coupled: lateral inhibition
  - the output of the neuron with maximum activation is set to one;
    all other to zero

$$y'_k = \begin{cases} 1 & \text{if } y_k > y_j \ \ \forall j \,.\, j \neq k \\ 0 & \text{else} \end{cases}$$

Clustering with Neural Networks

- the weights of the inputs of the winning neuron are adjusted as to move them towards observed sample

$$w'_{ij} = \begin{cases} w_{ij} + \eta(x_i - w_{ij}) & \text{for the winning neuron} \\ w_{ij} & \text{else} \end{cases}$$

- overall effect: moving the weights towards the center of gravity of the corresponding cluster
- problem: convergence
- other neural network approaches
  - self-organizing maps (SOM)
  - learning vector quantization (LVQ)

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Dependency Modelling

- prediction of events commonly occurring together
- market basket analysis: which items are often purchased together
    - placement of items in a store
    - layout of mail-order catalogues
    - targeted marketing campaigns
- association rules: rules of the form

$$a \wedge b \wedge \ldots \wedge c \rightarrow d \wedge e$$

- finding good combinations of premises is a combinatorial problem

Association Rules

- example data base:

trans-action	item
001	cola
001	chips
001	peanuts
002	beer
002	chips
002	cigarettes
...	...

trans-action	items
001	{chips, cola, peanuts}
002	{beer, chips, cigarettes}
003	{beer, chips, cigarettes, cola}
004	{beer, cigarettes}

Association Rules

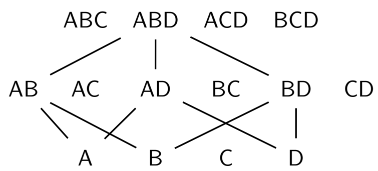
- set of n different items $I = \{x_j | j = 1, \ldots, n\}$
- itemset: $I_k \subseteq I$
- i-itemset: $I_k^i \subseteq I, \;\; |I_k^i| = i$
- transaction $T_k \subseteq I$
- data base: $D = \{(k, T_k) | k = 1, \ldots, m\}$
- support of an itemset: share of transactions which contain the itemset

$$s(I_i) = \frac{|\{T_k | I_i \subseteq T_k\}|}{|D|}$$

- frequent (strong, large) itemset: $s(I_i) \geq s_{min}$

Association Rules

- downward closure: every subset of a frequent itemset is also a frequent itemset



- every superset of a not frequent itemset is also a not frequent itemset

Association Rules

- association rule: $X \rightarrow Y, \quad X, Y \subseteq I, Y \cap X = \emptyset$
- support of a rule: share of transactions which contain both, premise and conclusion of the rule

$$s(X \rightarrow Y) = s(X \cup Y) = \frac{|\{T_k | X \cup Y \subseteq T_k\}|}{|D|} = p(XY)$$

- confidence of a rule: share of transactions supporting the rule from those supporting the premise

$$c(X \rightarrow Y) = \frac{s(X \cup Y)}{s(X)} = \frac{|\{T_k | X \cup Y \subseteq T_k\}|}{|\{T_k | X \subseteq T_k\}|} = p(Y|X)$$

Association Rules

- strong rule: high support + high confidence
- detection of strong rules: two pass algorithm

1. find frequent (strong, large) itemsets (Apriori)
    - necessary to generate rules with strong support
    - uses the downward closure
    - itemsets are ordered
2. use the frequent itemsets to generate association rules
    - find strong correlations in a frequent itemset

Association Rules

- Apriori: finding frequent itemsets of increasing size
  itemsets are ordered!
    - start with all itemsets of size one: I^1
    - select all itemsets with sufficient support
    - from the selected itemsets I^i generate larger itemsets I^{i+1}

$$is(\{i_1, \ldots, i_{n-2}, i_{n-1}\}) \wedge is(\{i_1, \ldots, i_{n-2}, i_n\})$$
$$\rightarrow is(\{i_1, \ldots, i_{n-2}, i_{n-1}, i_n\})$$

        - already blocks some of the non-frequent itemsets, but not all of them
    - remove those itemsets which still contain a non-frequent immediate subset
        - they cannot have enough support (downward closure)
    - continue until no further frequent itemsets can be generated

Association Rules

- example data base again
- assumption: minimum support $s_{min} = 0.5$

k	T_k
001	{chips, cola, peanuts}
002	{beer, chips, cigarettes}
003	{beer, chips, cigarettes, cola}
004	{beer, cigarettes}

I_k^1	#	$s(I_k^1)$
{chips}	3	0.75
{cola}	2	0.5
{peanuts}	1	0.25
{beer}	3	0.75
{cigarettes}	3	0.75

- no non-empty subsets

Association Rules

- 2-itemsets I_k^2

I_k^1	#	$s(I_k^1)$
{chips}	3	0.75
{cola}	2	0.5
{beer}	3	0.75
{cigarettes}	3	0.75

I_k^2	#	$s(I_k^2)$
{chips, cola}	2	0.5
{beer, chips}	2	0.5
{chips, cigarettes}	2	0.5
{beer, cola}	1	0.25
{cigarettes, cola}	1	0.25
{beer, cigarettes}	3	0.75

- no itemsets to prune

Association Rules

- 3-itemsets I_k^3

I_k^2	#	$s(I_k^2)$
{chips, cola}	2	0.5
{beer, chips}	2	0.5
{chips, cigar.}	2	0.5
{beer, cigar.}	3	0.75

I_k^3	#	$s(I_k^2)$
{beer, chips, cigar.}	2	0.5
{chips, cigar., cola}	1	0.25

Association Rules

- resulting frequent itemsets:

{beer, chips, cigarettes}
{chips, cola}
{chips, beer}
{chips, cigar.}
{beer, cigar.}
{beer}
{chips}
{cigarettes}
{cola}

Association Rules

- generation of strong association rules:
  - for all frequent itemsets I_j determine all nonempty subsets I_k for which

$$c = \frac{s(I_j)}{s(I_k)} \geq c_{min}$$

  - add a rule $I_k \rightarrow Y, \quad Y = I_j - I_k$ to the rule set
- e.g. $s(\{chips\}) = 0.75, s(\{cola\}) = 0.5,$ $s(\{chips, cola\}) = 0.5$

rule	confidence
{cola} → {chips}	1.00
{chips} → {cola}	0.67

Association Rules

- interesting association rules: only those for which the confidence is greater than the support of the conclusion

$$c(X \rightarrow Y) > s(Y)$$

- negative border:

$$\{I_k \mid s(I_k) < s_{min} \wedge \forall I_j \subset I_k \,.\, s(I_j) \geq s_{min}\}$$

used
  - to compute the set of frequent itemsets more efficiently
  - to derive negative association rules

Association Rules

- hierarchical Apriori algorithm
  - in addition to the base level of items, determine also frequent itemsets on a higher level in an is-a hierarchy

```
                food
             /        \
     beverages          snacks
       /   \            /    \
    cola   beer    peanuts   chips
```

  - sometimes regularities can only be found at higher levels of abstraction

Association Rules

- the Apriori algorithm requires several scans of the database
- goal: reducing the number of scans
- partitioned Apriori: two scans
  - 1st scan: partition the database and compute locally frequent itemsets on the partitions
  - 2nd scan: determine the support of all locally frequent itemsets
  - heuristics: if an itemset is globally frequent it will be so locally in at least one partition
    → second scan deals with a superset of possible itemsets

Association Rules

- sampling: multiple scans
  - 1st scan: take a sample and compute frequent itemsets
  - 2nd scan: count their support and the support for their immediate supersets
  - if the itemset is at the negative border
    - all frequent itemsets have been found
    - else check supersets of the itemsets for being at the negative border in subsequent scans

Association Rules

- incremental update: scan only the added transactions, whether they
  - invalidate a former frequent itemset, or
  - introduce new frequent itemsets

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Summarization

- extraction of representative information about the database
- simple decriptions: characterizations, generalizations
  - point estimations: mean, variance
  - confidence intervals
  - regression functions
  - cluster with prototypical examples
  - association rules

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Temporal Data Bases

- snapshot databases: no support for temporal data
- transaction time databases: tuples or attribute values are timestamped when inserted
- valid time databases: tuples or attribute values can be annotated for the time range in which they are valid
- bitemporal databases: both types of temporal information are supported

Sequential Structures

- time is inherently sequential
- models for capturing sequential structures
  - Finite State Automata
  - Markov Models
  - Hidden Markov Models
- all require supervised training

Time Series Analysis

- trend detection: smoothing by a moving average
- prediction: fitting the coefficients of a (linear) equation
- (seasonal) cycle detection: autocorrelation
- outlier detection
- event detection: classification based on preceding data points

Pattern Detection

- longest common subsequence
  - fraud detection
  - genomic analysis
  - failure prediction
  - desaster prediction (vulcano eruptions, earthquakes, floodings)
- for categorial data: extension of Apriori to sequences
- flexible match required
  - extension of the similarity measures to sequences
  - special case: elastic match (dynamic time warping)
  - general case: match with transpositions
- for numerical data: (Hidden) Markov Models

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Visualization

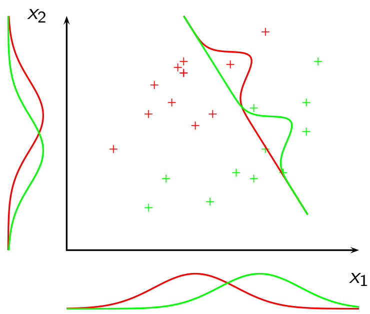
- seeing is the construction of a mental image
  - abstraction: identification of objects, assigning properties
  - generalization: summarized information about many data points
- basic graph types
  - bar charts
  - histograms (distributions)
  - line charts
  - pie charts
  - scatter plots

Visualization

- problem: limited dimensionality
  - two (three) basic dimensions
  - overlay of multiple graphs
  - color
  - texture
  - shape
  - animation
- combination of visualisation techniques with data cube operations
- interactive exploration of data: browsing

Visualization

- rolling the dice is not always sufficient

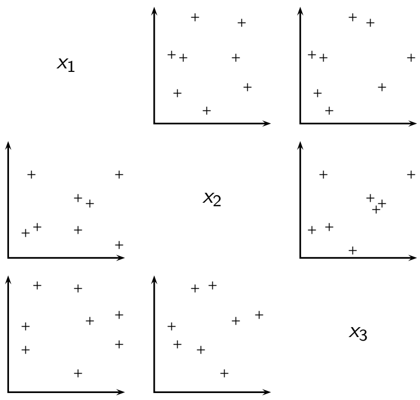


Multi-Dimensional Visualization

- scatter-plot matrix
- parameter stacks
- parallel coordinates
- star display
- radial visualization

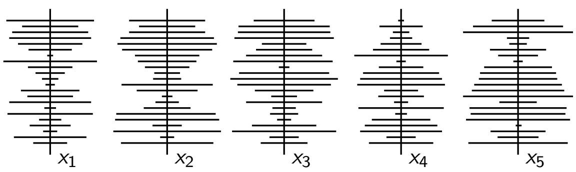
Scatter-Plot Matrix

- $n \times n$-matrix of all combinations of two dimensions

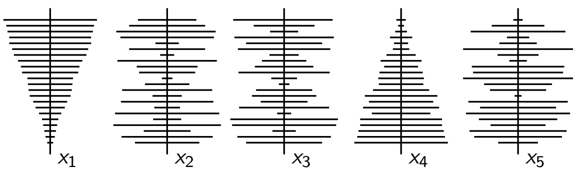


Parameter Stacks

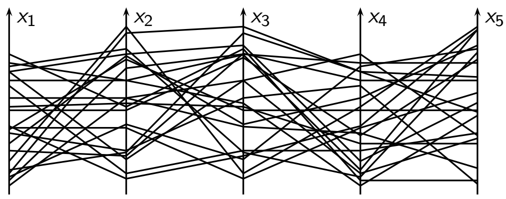
- data plots on vertical lines as centered horizontal lines



- exploring data by sorting along a dimension



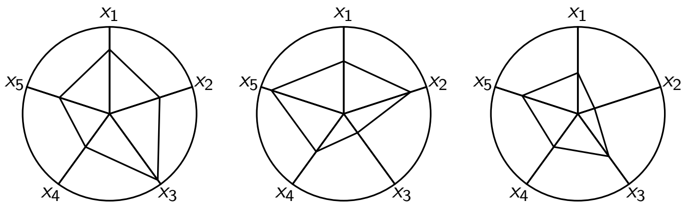
Parallel Coordinates



- exploring data by investigating neighborhood relationships between dimensions
  - rearranging

Star Display

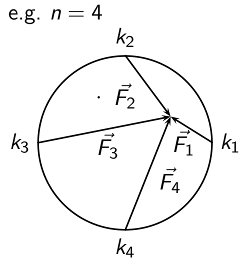
- radial version of parallel coordinates



- only for the display of few data points

Radial Visualization

- attraction-based: forces proportional to the n dimensions pull the point towards the dimension anchors
- equilibrium: forces must sum up to 0
- mapping the n-dimensional space into a two dimensional one $(k_1, k_2, k_3, k_4, ..., k_n) \mapsto (x, y)$
- e.g. $n = 4$



$$\vec{F}_1 + \vec{F}_2 + \vec{F}_3 + \vec{F}_4 = 0$$

Radial Visualisation

$$k_1 \begin{pmatrix} 1-x \\ 0-y \end{pmatrix} + k_2 \begin{pmatrix} 0-x \\ 1-y \end{pmatrix} + k_3 \begin{pmatrix} -1-x \\ 0-y \end{pmatrix} + k_4 \begin{pmatrix} 0-x \\ -1-y \end{pmatrix} = 0$$

$$k_1 - k_1 \cdot x - k_2 \cdot x - k_3 - k_3 \cdot x - k_4 \cdot x = 0$$

$$-k_1 \cdot y + k_2 - k_2 \cdot y - k_3 \cdot y - k_4 - k_4 \cdot x = 0$$

$$k_1 - k_3 - x(k_1 + k_2 + k_3 + k_4) = 0$$

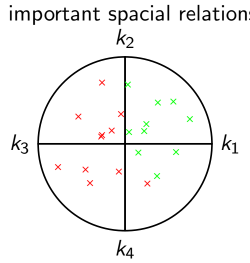
$$k_2 - k_4 - y(k_1 + k_2 + k_3 + k_4) = 0$$

$$x = \frac{k_1 - k_3}{k_1 + k_2 + k_3 + k_4}$$

$$y = \frac{k_2 - k_4}{k_1 + k_2 + k_3 + k_4}$$

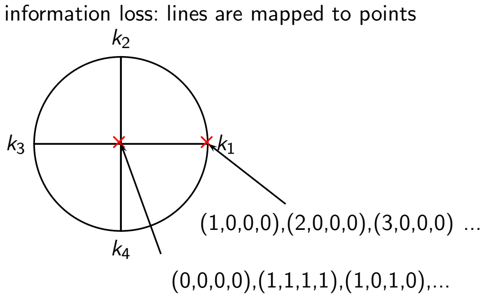
Radial Visualization

- important spacial relationships are preserved: e.g. class separation



Radial Visualisation

- information loss: lines are mapped to points



Sonification

- hearing data
- auditory channel is inherently multidimensional
  - volume, rhythm, pitch, harmony, polyphony, sound color, ...
- approaches
  - audification
  - sound mapping
  - model-based sonification

Sonification

- audification: direct mapping of time-series data to sound patterns
  - detection of rhythmic patterns
  - traffic density
- sound mapping: controlling sound synthesis parameter by data items
  - high-dimensional data can be presented
- model-based sonification: excitation of an oscillating model by data items
  - energetically coupled particles, growing neural gas
  - interactive exploration of the (auditory) system response
  - linear structures in a high-dimensional space can be identified