Data Mining, Lecture 1

Introduction & Distance Function

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Course organization: (administrative part)

- For all correspondence concerning the course use email sven.nomm@ttu.ee Please avoid using phone.
- Grading:
  - 3x mandatory closed book tests. Each test gives 10% of the final grade. For each test one make-up attempt.
  - 3x mandatory home assignments (Computational assignment + short write up.) 10% of the final grade each. Assignments are accepted up to one week after the deadline with the penalty of 10% for each day except Saturday and Sunday.
  - final exam (gives 40 % of the final grade): Written report on assigned topic + discussion with lecturer. Prerequisites:
    - ★ all 3 closed book tests are accepted (graded as 51 or higher)
    - ★ all 3 home assignments are accepted (graded as 51 or higher)
- **No Plagiarism in any of assignments and final project!!!**. You should cite all the references, including software and extra libraries. The student should be able to explain the meaning of all the computations performed, interpret and present the results.

Course organization: Grading *vs.* expected knowledge

- **Excellent 91 -100** Able to apply all the methods and techniques, thought during the course, on practice. Interpret the results and explain theoretical foundations of the applied techniques Discuss achieved results with respect of possible further analysis. Able to learn new techniques independently and apply them on practice.
- **Very Good 81 -90** Able to apply all the methods and techniques, thought during the course, on practice. Interpret the results and explain theoretical foundations of the applied techniques. Discuss achieved results with respect of possible further studies.
- **Good 71 -80** Able to apply all the methods and techniques, thought during the course, on practice, interpret the results and explain theoretical foundations of the applied techniques.
- **Satisfactory 61-70** Able to apply all the methods and techniques, thought during the course, on practice. Interpret the results.
- **Acceptable 51-60** Able to apply all core methods and techniques, thought during the course, on practice. Interpret the results.

References

The structure of the present course, main notations and definitions are inherited from [1]. [7] provides basic knowledge of "R" for the data mining assignments. Implementation of different data mining algorithms in "R" is discussed by [3]. Some data mining methods are borrowed from the neighbouring fields of research, such as Machine Learning [2], Pattern Recognition [6] and Feature Extraction [4]. Lectures related to the networked data mining are based on [5].

[1] C.C. Aggarwal. *Data Mining: The Textbook*. Springer International Publishing, 2015.

[2] A. Agresti. *Categorical Data Analysis*. Wiley Series in Probability and Statistics. Wiley, 2013.

[3] P. Cichosz. *Data Mining Algorithms: Explained Using R*. Wiley, 2015.

[4] I. Guyon, S. Gunn, M. Nikravesh, and L.A. Zadeh. *Feature Extraction: Foundations and Applications*. Studies in Fuzziness and Soft Computing. Springer Berlin Heidelberg, 2008.

[5] E.D. Kolaczyk and G. Csárdi. *Statistical Analysis of Network Data with R*. Use R! Springer New York, 2014.

[6] S. Theodoridis and K. Koutroumbas. *Pattern Recognition*. Elsevier Science, 2008.

[7] G. Williams. *Data Mining with Rattle and R: The Art of Excavating Data for Knowledge Discovery*. Use R! Springer New York, 2011.

Course organization: administrative part (continued)

- You are expected to attend the lectures and practices. Lecture slides do not contain all the information. Also, this is the place where you can gain experience!
- Consultations: By appointment only! Please do not hesitate to ask if you need consultation.
- It is advisable to write your own notes!
- Mind academic 15 min!
- Many concepts introduced during the course require understanding of the probability theory and statistics.
- "R" and some related packages will be used to perform computational part of the assignments.
- Any questions?

It is advisable to refresh your knowledge of:

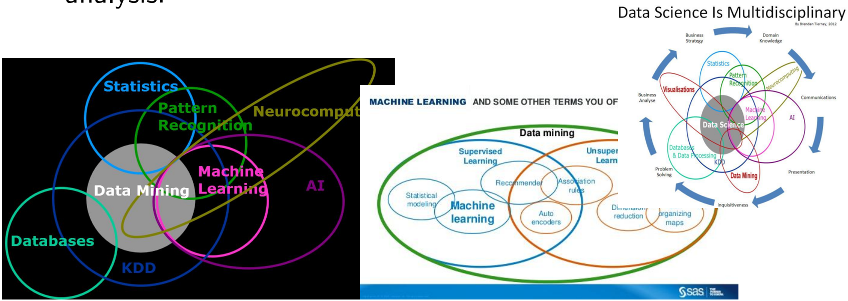
- Mathematics (calculus and linear algebra).
- Statistics.
- Programming.

Course main topics(tentative)

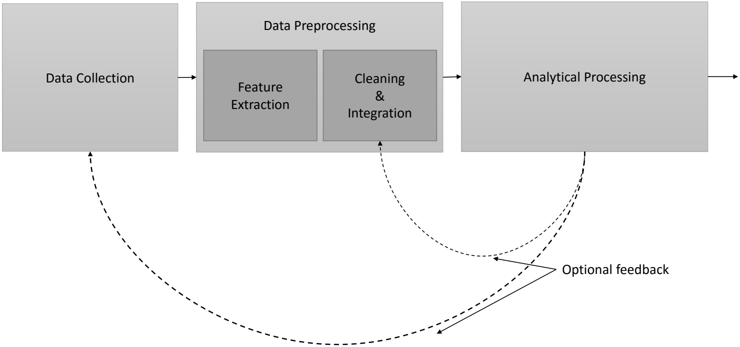
- What data mining is?
- Data mining vs. Machine learning vs. ?
- Four "super problems" of data mining:
  - Clustering
  - Classification
  - Association pattern mining
  - Outlier analysis and anomalies detection.
- Main Topics
  - Data types and Data Preparation
  - Similarity and Distances, Association Pattern Mining
  - Cluster Analysis, Classification, Outlier analysis
  - Data streams, Text Data, Time Series, Discrete Sequences
  - Spatial Data, Graph Data, Web Data, Social Network Analysis
  - Privacy-Preserving Data Mining

What data mining is?

- Aggarwal: "Data mining is the study of collecting, cleaning, processing, analyzing and gaining useful insides from the data."
- Williams: "Data mining is the art and science of intelligent data analysis."



The Data Mining Process



Attribute, Feature, Dimensionality

- **Widely used explanation** Different measured properties of the process are referred as *features*, *attributes* or *dimensions*.
- In order to avoid confusion, here and after, single measured property of the process will be referred as *attribute*, sets or tuples of attributes will be referred as *features*. Note! That feature may contain just one attribute therefore attribute is always a feature but not vice verse! *Dimensionality* is the property of the process describing number of attributes.

Data Types

- **Nondependency-oriented data** The simplest form of data usually refers to multidimensional data.
  - Quantitative multidimensional data
  - Binary and set data
  - Text data
- **Dependency-oriented data**
  - Time-series data
  - Discrete sequences and strings
  - Spatial data
  - Network and graph data

Nondependency-oriented data / multidimensional data

Definition (1)

Multidimensional Data: *A multidimensional data set $\mathcal{D}$ is a set of n records, $\bar{X}_1 \dots \bar{X}_n$, such that each record $\bar{X}_i$ contains a set of features denoted $(x_i^1 \dots x_i^d)$.*

- **Quantitative multidimensional data.** If each element x_i^j in Definition 1 is quantitative, then corresponding data set $\mathcal{D}$ is referred as *quantitative multidimensional* data.
- **Categorical and mixed attribute data.** If each element x_i^j in Definition 1 categorical (unordered discrete), then corresponding data set $\mathcal{D}$ is referred as *unordered discrete-valued* or *categorical*
- **Binary and set data.** may be considered as a special case of either multidimensional categorical data (each attribute may take only one of two values) or multidimensional quantitative data (ordering exists between two values).
- **Text data** belong to the dependency oriented data types but its vector-space representation (words correspond to attributes and their frequencies to the values of these attributes).

Dependency-Oriented Data

It is assumed that at least between two records of the data set explicit or implicit relations may exist.

- **Time-series data**

Definition

A time series of length n and dimensionality d is a $n \times d$ matrix Y, where each string corresponds to the certain time instance and each row corresponds to a certain numeric feature.

- **Discrete sequences and strings.** Categorical analog of time-series data. Each element of the matrix Y may take discrete or categorical value.

Dependency-Oriented Data

- **Spatial data**

Definition

Spatial data: *A d - dimensional spatial data record contains d behavioral attributes and one or more contextual attributes containing the spatial location. d- dimensional spatial data set is a set of d -dimensional records $\bar{X}_1 \dots \bar{X}_n$, together with the set of locations $L_1 \dots L_n$, such that the record $\bar{X}_i$ is associated with the location L_i.*

Important subclass spatiotemporal data.

- **Network and graph data**

Definition

A network $G = (N, A)$ is defined by the set of nodes N and a set of edges A, where edges represent th relationships between the nodes.

In some cases an attribute sets $\bar{X}_i$ and $\bar{Y}_{i,j}$ may be associated with node i and edge i, j correspondingly.

Problems (major building blocks)

- **Association Pattern Mining** Frequent pattern mining

Definition

Given a binary $n \times d$ data matrix $\mathcal{D}$, determine all subsets of columns such that all values in this columns take on the value of 1 for at least a fraction s of the rows in the matrix.

- **Data Clustering**

Definition

Given a data matrix or database $\mathcal{D}$, partition its rows (records) into sets $C_1 \dots C_k$ such the rows (records) in each cluster are similar to one another.

- **Outlier Detection**

Definition

Given a data matrix $\mathcal{D}$, determine the rows that are "very" different from the remaining rows of the matrix

Problems (major building blocks)

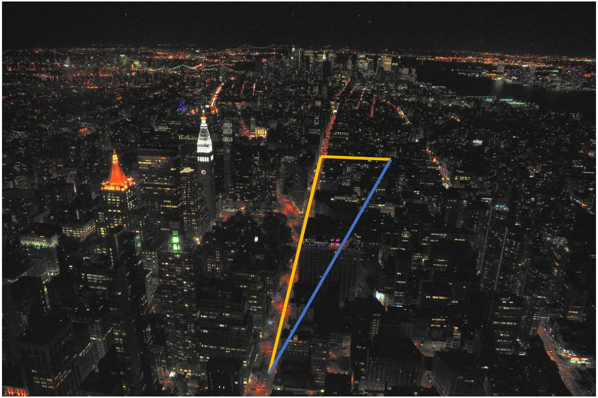
- **Data Classification**

Definition

Given an $n \times d$ training data matrix (database) $\mathcal{D}$, and a class label volume in $\{1, \ldots, k\}$ associated with each of the n rows (records in case of database) in $\mathcal{D}$, create a training model $\mathcal{M}$ which can be used to predict the class label of a d dimensional row (record) $\bar{Y} \notin \mathcal{D}$.

- **Complex Data Types**
- **Scalability Issues**

Distance ?



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This is the distance used to compute the price of a taxi ride

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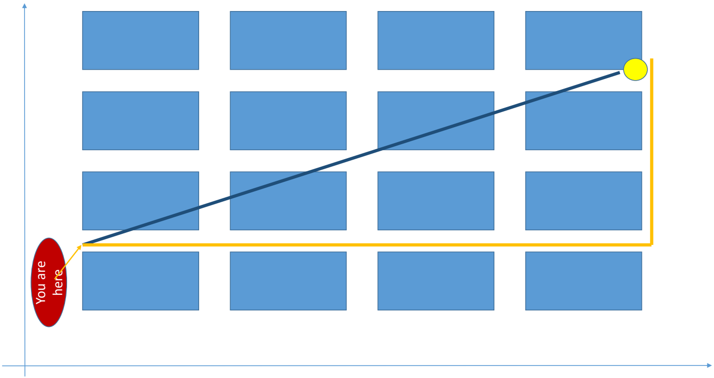
Actual distance between the starting end ending points of your journey

Distance ?



Real world distances

- Euclidean distance

$$S(x,y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

- Manhattan distance also referred as city block distance or taxicab distance

$$S(x,y) = \sum_{i=1}^{n} \mid x_i - y_i \mid$$

Let us suppose that $(2,3)$ are the coordinates of the starting point and (11,14) are the coordinates of the destination. Then Euclidian distance between the starting point and destination is: 14.21. At the same time Manhattan distance is 20.

Similarity or Distance

Problem statement: *Given two objects $\mathcal{O}_1$ and $\mathcal{O}_2$, determine a value of the similarity between two objects*

Distance function

Distance function is one of most fundamental notions in Machine learning and Data mining. Formally defined in pure mathematics as *metric* function. It provides measure of similarity or distance between two elements.

Definition

A function $S : X \times X \to \mathbb{R}$ is called metric if for any elements x, y and z of X the following conditions are satisfied.

1. Non-negativity or separation axiom
$$S(x, y) \geq 0$$
2. Identity of indiscernible, or coincidence axiom
$$S(x, y) = 0 \Leftrightarrow x = y$$
3. Symmetry
$$S(x, y) = S(y, x)$$
4. Subadditivity or triangle inequality
$$S(x, z) \leq S(x, y) + S(y, z)$$

Distance function: Examples 1 (Most common distance functions)

- Euclidean distance

$$S(x,y)=\sqrt{\sum_{i=1}^{n}(x_i-y_i)^2}$$

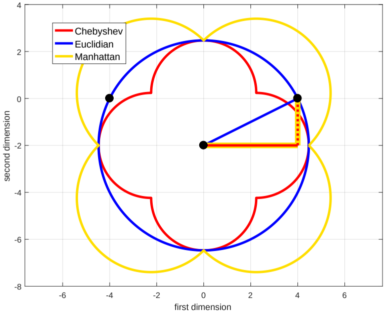
- Manhattan distance also referred as city block distance or taxicab distance

$$S(x,y)=\sum_{i=1}^{n}\mid x_i-y_i\mid$$

- Chebyshev distance

$$S(x,y)=\max_i\bigl(\mid x_i-y_i\mid\bigr)$$

Distance function: Examples 2



Euclidean distance

$$S(x,y)=\sqrt{\sum_{i=1}^{n}(x_i-y_i)^2}$$

Manhattan distance

$$S(x,y)=\sum_{i=1}^{n}\mid x_i-y_i\mid$$

Chebyshev distance

$$S(x,y)=\max_i\left(\mid x_i-y_i\mid\right)$$

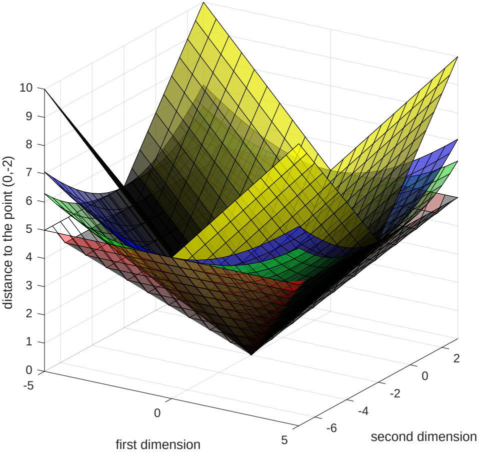
Distance function:Examples 3 Minkowsky distance

$$S(x,y) = \Big(\sum_{i=1}^{d} \mid x_i - y_i \mid^p\Big)^{1/p}$$

- $p < 1$ triangle inequality is violated, therefore for the values of p smaller than one, equation above is not a distance function.
- $p = 1$ case of Manhattan distance.
- $p = 2$ case of Euclidian distance.
- $p \to \infty$ case of Chebyshev distance.

Distance function: Examples 4

3D representation of the Minkovski distances for different values of parameter p. $p = 1$ - yellow surface, Manhattan; $p = 2$ - blue surface, Euclidean,; $p = 3$ - green surface; $p \to \infty$ - red surface, Chebyshev.

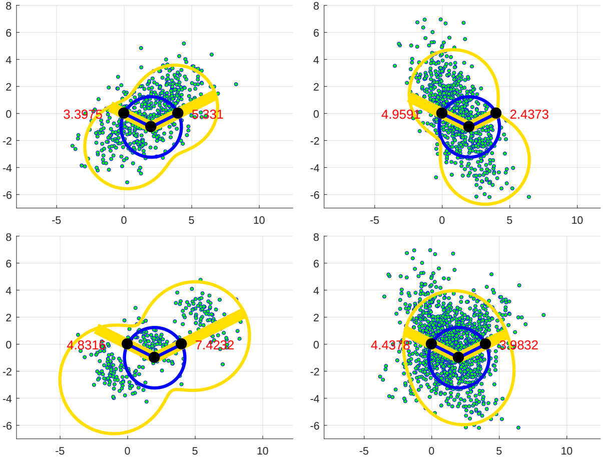


Distance function: Examples 5

Mahalanobis distance

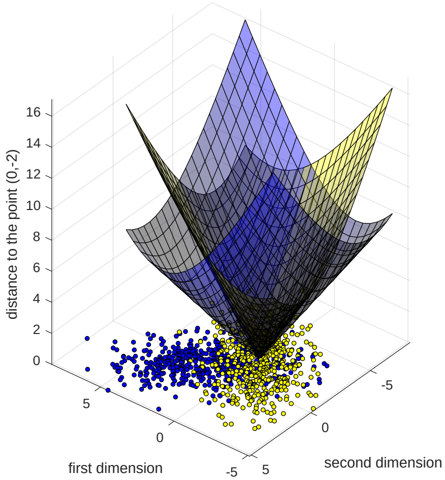
$$S(x,y) = \sqrt{(x-y)^T C^{-1} (x-y)}$$

where C is the covariance matrix. Takes into account impact of data distribution.



Distance function: Examples 6

- Impact of the rotation of underlying data set.



Distance function: Examples 7

- Canberra distance
$$S(x,y)=\sum_{i=1}^{n}\frac{|x_i-y_i|}{|x_i|+|y_i|}$$
weighted version of Manhattan distance.
- Cosine distance Cosine similarity is the measure of the angle between two vectors
$$S_c(x,y)=\frac{x\cdot y}{\|x\|\|y\|}$$
Usually used in high dimensional positive spaces, ranges from -1 to 1. Cosine distance is defined as follows
$$S_C(x,y)=1-S_c(x,y)$$

Distance function: Examples 8

- Levenshtein or SED distance. SED - minimal number of single -charter edits required to change one string into another. Edit operations are as follows:
  - insertions
  - deletions
  - substitutions
- SED(delta, delata)$=1$ delete "a" or SED(kitten,sitting)$=3$: substitute "k" with "s",substitute "e" with "i", insert "g".
- Hamming distance Similar to Levenshtein but with substitution operation only. Frequently used with categorical and binary data.
- Specialized similarity measures Distance and similarity functions applicable to the graphs, temporal data etc. These topics are left outside of the framework of the present course.

Impact of High Dimensionality (Curse of Dimensionality)

Curse of dimensionality - term introduced by Richard Bellman. Referred to the phenomenon of efficiency loss by distance based data-mining methods. Let us consider the following example.

- Consider the unit cube in d - dimensional space, with one corner at the origin.
- What is the Manhattan distance from the arbitrary chosen point inside the cube to the origin?

  $$S(\bar{0}, \bar{Y}) = \sum_{i=1}^{d} (Y_i - 0)$$

  Note that Y_i is random variable in $[0, 1]$
- The result is random variable with a mean $\mu = d/2$ and standard deviation $\sigma = \sqrt{d/12}$
- The ratio of the variation in the distances to the mean value is referred as *contrast*

  $$G(d) = \frac{S_{max} - S_{min}}{\mu} = \sqrt{\frac{12}{d}}$$

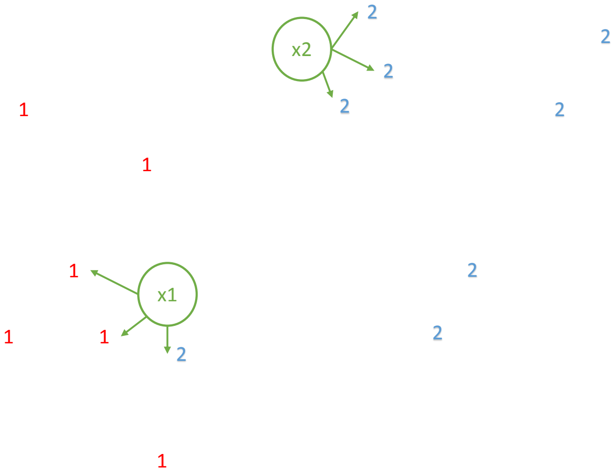
k-nearest neighbour (k-NN) classification

- Let N be a labeled set of points belonging to c different classes such that

$$\sum_{i=1}^{c} N_i = N$$

- Classification of a given point x
  - Find k - nearest points to the point x.
  - Assign x the majority label of neighbouring (k-nearest) points

Example



L_p norms

- The real valued function f defined in a vector space V over the subfield F is called a norm if for any $a \in F$ and all $u, v \in V$ it satisfies following three conditions
  - $f(av) = \mid a \mid f(v)$
  - $f(u+v) \leq f(u) + f(v)$
  - $f(v) = 0 \Rightarrow v = 0$
- L_p is defined as follows

$$S(\bar{X}\bar{Y}) = \left(\sum_{i=1}^{d} \mid x_i - y_i \mid^p\right)^{\frac{1}{p}}$$

- In case of $p = 1$ we are dealing with already known to you Manhattan distance. In case of $p = 2$ Euclidean.

Impact of Domain-Specific Relevance

There are cases when some features are more important than the others. Generalized L_p distance is most suitable in such cases.

$$S(x,y) = \Big(\sum_{i=1}^{d} a_i \mid x_i - y_i \mid^p\Big)^{1/p}$$

This distance is frequently referred as *Minkowski distance*