Clustering Algorithms

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WS 2015/16

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Introduction

Clustering techniques for data management and analysis that classify/group given set of objects into categories/subgroups or clusters

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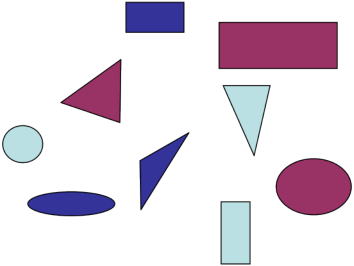
Goals

1. find structures in large set of objects/data
2. simplify large data sets

Example



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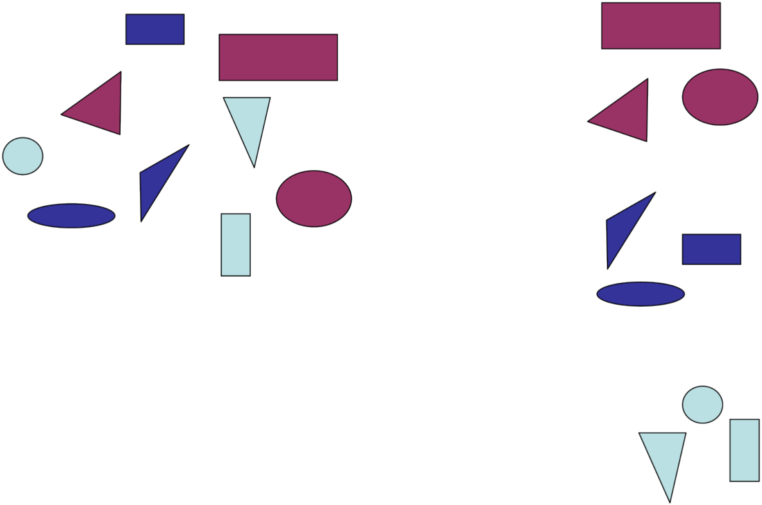

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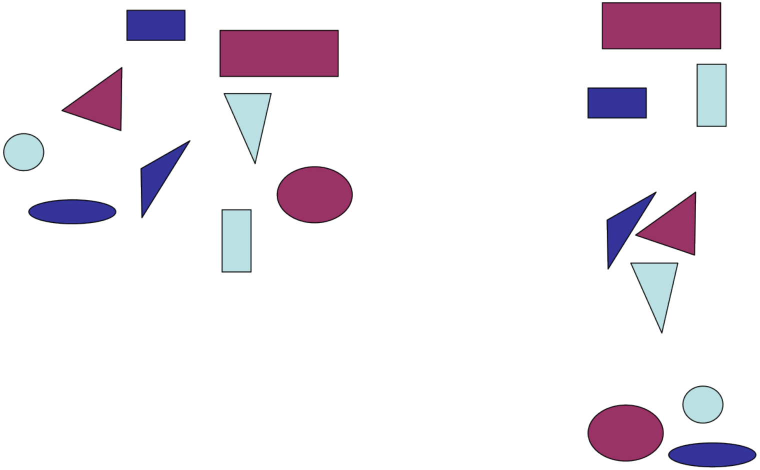
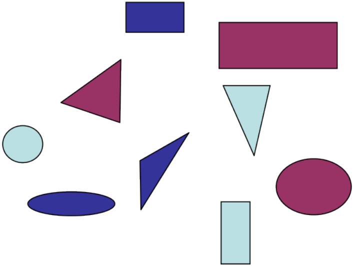
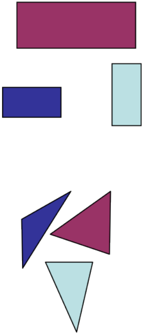
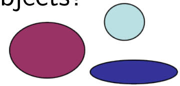






How do we measure similarity/dissimilarity of objects?



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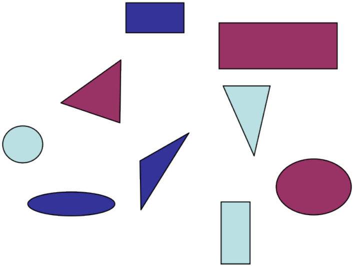
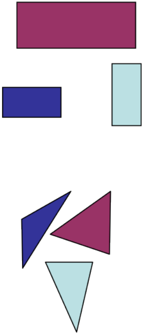
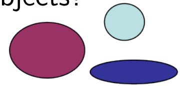




How do we measure similarity/dissimilarity of objects?

How do we measure quality of clustering?



Application areas

1. information retrieval

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2. data mining

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3. machine learning

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8. bioinformatics
9. speech recognition.

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- improvements to these heuristics
- various theoretical results about clustering, including NP-hardness results and approximation algorithms
- general techniques to improve the efficiency of heuristics and approximation algorithms, i.e. dimension reduction techniques.

Organization

Information about this course
http://www.cs.uni-paderborn.de/fachgebiete/ag-bloemer/lehre/2015/ws/clusteringalgorithms.html

Here you find

- announcements
- handouts
- slides
- literature

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- There is only one tutorial, Thursday 13:00 -14:00.
- It starts next week.

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Prerequisites

- design and analysis of algorithms
- basic complexity theory
- probability theory and stochastic
- some linear algebra

Objects

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- features continuous or binary

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- objects described as elements in $\mathbb{R}^d$ or $\{0,1\}^d$

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Objects

- objects described by d different features
- features continuous or binary
- objects described as elements in $\mathbb{R}^d$ or $\{0,1\}^d$
- objects from $M \subseteq \mathbb{R}^d$ or $M \subseteq \{0,1\}^d$

Definition 1.1

$D : M \times M \to \mathbb{R}$ *is called a distance function, if for all* $x, y, z \in M$

- $D(x, y) = D(y, x)$ *(symmetry)*
- $D(x, y) \geq 0$ *(positivity),*

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D is called a metric, if in addition,

- $D(x, y) = 0 \Leftrightarrow x = y$ *(reflexivity)*
- $D(x, z) \leq D(x, y) + D(y, z)$ *(triangle inequality)*

Example 1.2 (Euclidean distance)

$M = \mathbb{R}^d$,

$$D_{l_2}(x, y) = \|x - y\|_2 = \Big(\sum_{i=1}^{d} |x_i - y_i|^2\Big)^{\frac{1}{2}},$$

where $x = (x_1, \ldots, x_d)$ *and* $y = (y_1, \ldots, y_d)$.

Example 1.3 (Squared Euclidean distance)

$M = \mathbb{R}^d$,

$$D_{l_2^2}(x, y) = \|x - y\|_2 = \sum_{i=1}^{d} |x_i - y_i|^2,$$

where $x = (x_1, \ldots, x_d)$ *and* $y = (y_1, \ldots, y_d)$.

Example 1.4 (Minkowski distances, l_p-norms)

$M = \mathbb{R}^d$, $p \geq 1$,

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Example 1.5 (maximum distance)

$M = \mathbb{R}^d$,

$$D_{l_\infty}(x,y) = \|x-y\|_\infty = \max_{1\leq i\leq d} |x_i - y_i|.$$

Example 1.6 (Pearson correlation)

$M = \mathbb{R}^d$,

$$D_{Pearson}(x,y) = \frac{1}{2}\left(1 - \frac{\sum_{i=1}^{d}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{d}(x_i - \bar{x})^2 \sum_{i=1}^{d}(y_i - \bar{y})^2}}\right),$$

where $\bar{x} = \frac{1}{d}\sum x_i$ *and* $\bar{y} = \frac{1}{d}\sum y_i$.

Example 1.7 (Mahalanobis divergence)

$A \in \mathbb{R}^{d \times d}$ *positive definite, i.e.* $x^T A x > 0$ *for* $x \neq 0$, $M = \mathbb{R}^d$,

$$D_A(x, y) = (x - y)^T A (x - y)$$

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Example 1.8 (Itakura-Saito divergence)

$M = \mathbb{R}^d_{>0}$,

$$D_{IS}(x, y) = \sum \frac{x_i}{y_i} - \ln\left(\frac{x_i}{y_i}\right) - 1.$$

Example 1.9 (Kullback-Leibler divergence)

$M = S^d := \{x \in \mathbb{R}^d : \forall i : x_i \geq 0, \sum x_i = 1\}$,

$$D_{KLD}(x, y) = \sum x_i \ln(x_i / y_i),$$

where by definition $0 \cdot ln(0) = 0$.

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Example 1.10 (generalized KLD)

$M = \mathbb{R}^d_{\geq 0}$,

$$D_{KLD}(x, y) = \sum x_i \ln(x_i / y_i) - (x_i - y_i),$$

Definition 1.11

$S : M \times M \to \mathbb{R}$ is called a similarity function, if for all $x, y, z \in M$

- $S(x, y) = S(y, x)$ *(symmetry)*
- $0 \leq S(x, y) \leq 1$ *(positivity),*

S is called a metric, if in addition,

- $S(x, y) = 1 \Leftrightarrow x = y$ *(reflexivity)*
- $S(x, y)S(y, z) \leq \big(S(x, y) + S(y, z)\big)S(x, z)$ *(triangle inequality)*

Example 1.12 (Cosine similarity)

$M = \mathbb{R}^d$,

$$S_{CS}(x,y) = \frac{x^T y}{\|x\|\|y\|} \quad or$$

$$\bar{S}_{CS}(x,y) = \frac{1 + S_{CS}(x,y)}{2}$$

Similarity for binary features

Let $x, y \in \{0,1\}^d$, then

$$n_{b\bar{b}}(x,y) := \left|\{1 \le i \le d : x_i = b, y_i = \bar{b}\}\right|$$

and for $w \in \mathbb{R}_{\ge 0}$

$$S_w(x,y) := \frac{n_{00}(x,y) + n_{11}(x,y)}{n_{00}(x,y) + n_{11}(x,y) + w\big(n_{01}(x,y) + n_{10}(x,y)\big)}.$$

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Popular: $w = 1, 2, \frac{1}{2}$.

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Example 1.13 (matching coefficient)

$$w = 1, S_{mc}(x,y) = \frac{n_{00}(x,y) + n_{11}(x,y)}{d}.$$

Similarity for binary features

$$\bar{S}_w(x, y) := \frac{n_{11}(x, y)}{n_{11}(x, y) + w\big(n_{01}(x, y) + n_{10}(x, y)\big)}$$

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Popular: $w = 1, 2, \frac{1}{2}$.

Example 1.14 (Jaccard coefficient)

$$w = 1, S_{Jacard}(x,y) = \frac{n_{11}(x,y)}{n_{11}(x,y) + n_{01}(x,y) + n_{10}(x,y)}.$$

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