

9.1 Linear Clustering

Machine Learning 1: Foundations

Marius Kloft (TUK)

Recap

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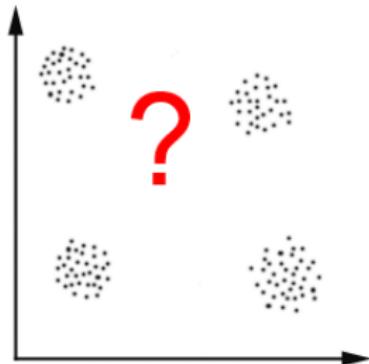
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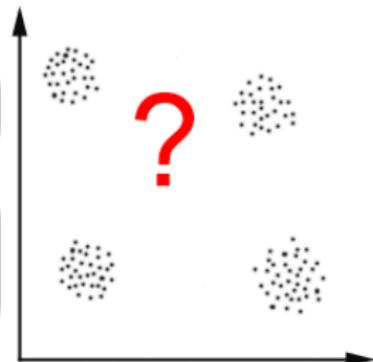
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But what if there are no labels given?

This setting is called
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Today and Next Week

Definition

Unsupervised learning is the area of machine learning where

- ▶ we are given inputs $x_1, \dots, x_n \in \mathbb{R}^d$
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What could be interesting tasks in unsupervised learning?

1. Anomaly Detection

Detect unusual data points

- ▶ i.e., that deviate strongly from the previously seen ones

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Rare events

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Attacks on networks

2. Density Estimation and Generative Models

Learn the **law** by which nature has generated the data



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And use it to **generate** new examples!



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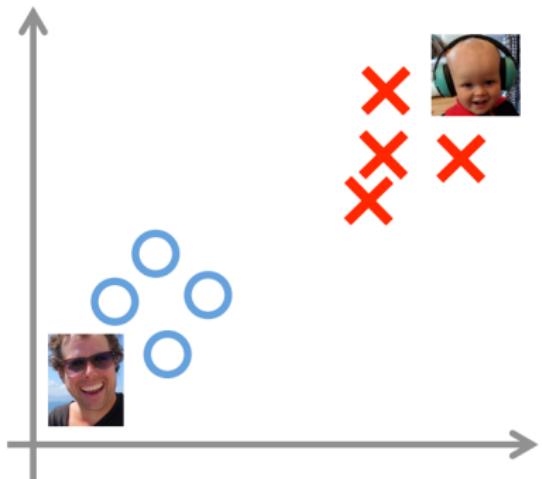
And use it to **generate** new examples!



We will learn in **ML2** how this works

3. Dimensionality Reduction (**Next Week!**)

Compress data into lower-dimensional representation

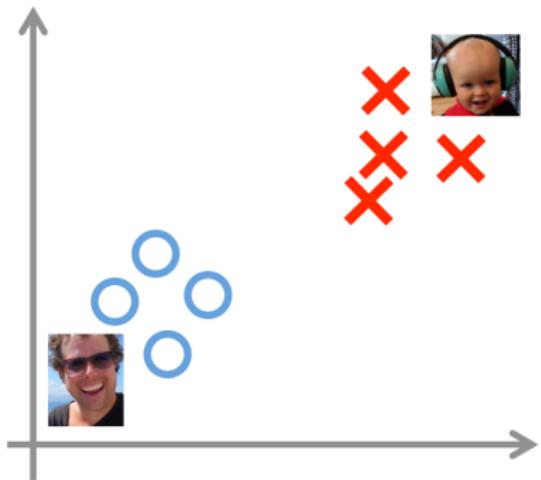


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Compress data into lower-dimensional representation

Applications:

- ▶ data visualization
- ▶ data de-noising



4. Clustering

Today!

Contents of this Class

Clustering

- 1 Linear Clustering
- 2 Non-linear Clustering
- 3 Hierarchical Clustering

1 Linear Clustering

2 Non-linear Clustering

3 Hierarchical Clustering

What is Clustering?

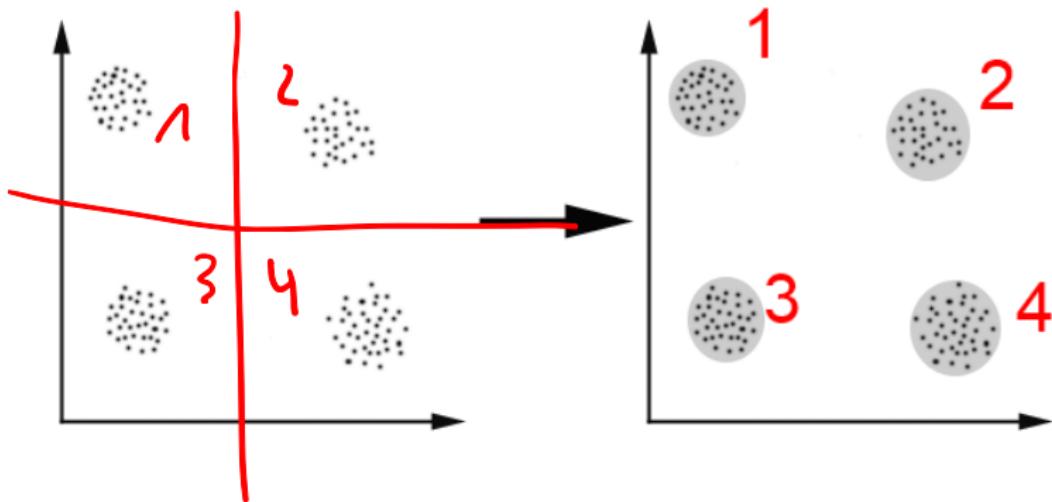
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Clustering is the process of organizing objects into groups—called **clusters**—whose members are similar in some way.

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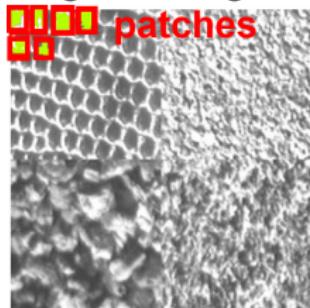
Example: Image Segmentation

Original image:

segmented image

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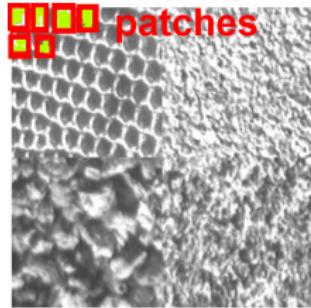


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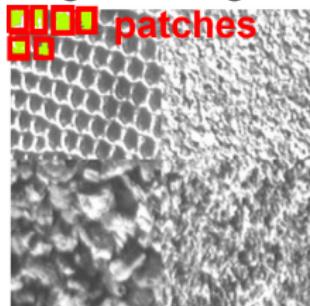
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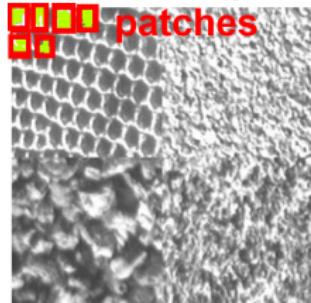
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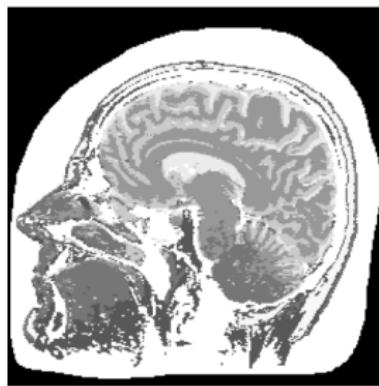
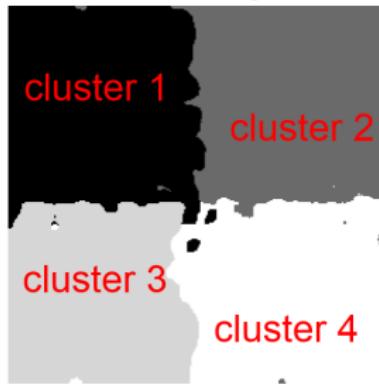
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More examples

- **Recommender systems:** organizing products and customers into groups that are similar



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- ▶ **Social networks:** cluster users into groups that have similar interests/preferences



More examples

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- ▶ **Social networks:** cluster users into groups that have similar interests/preferences



- ▶ **WWW document classification:** organize webpages (e.g., news articles) into clusters with similar content (sports, economics, ...)



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Big problem:

- ▶ evaluation of results!

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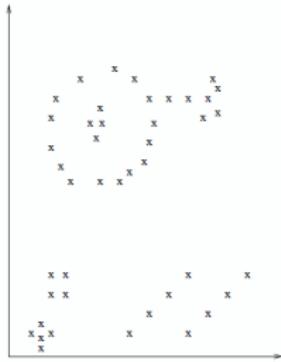
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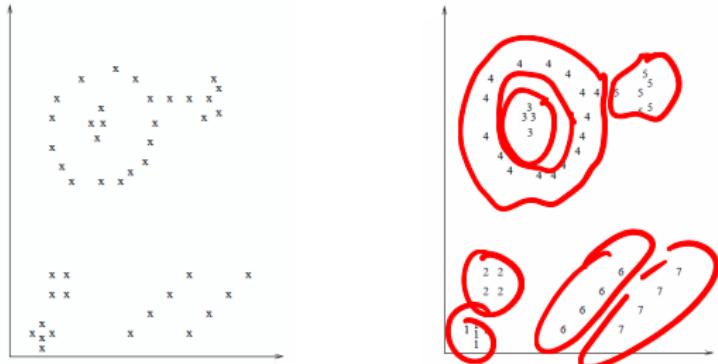


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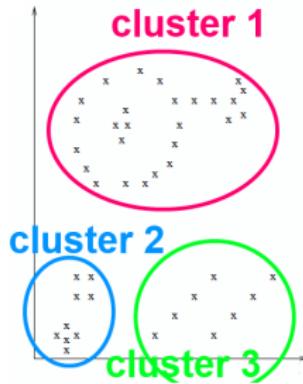
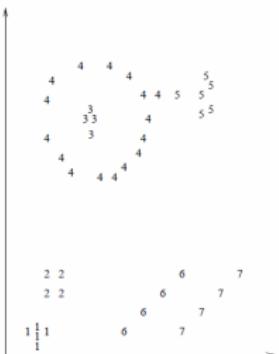
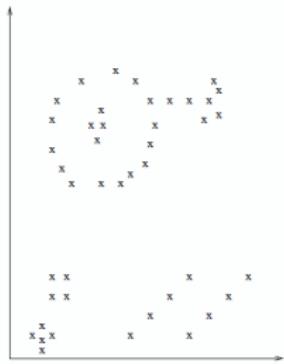


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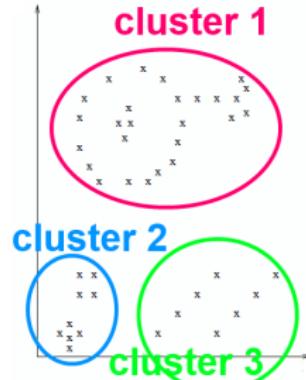
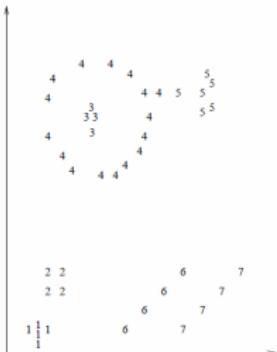
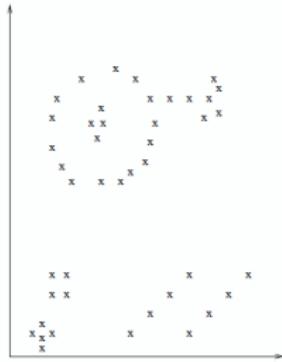


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7 clusters

vs.

3 clusters

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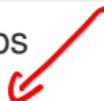
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cluster 1	cluster 2	cluster 3	cluster 4
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Arts Budgets Child Education

NEW
FILM
SHOW
MUSIC
MOVIE
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BEST
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FIRST
YORK
OPERA
THEATER
ACTRESS
LOVE

MILLION
TAX
PROGRAM
BUDGET
BILLION
FEDERAL
YEAR
SPENDING
NEW
STATE
PLAN
MONEY
PROGRAMS
GOVERNMENT
CONGRESS

CHILDREN
WOMEN
PEOPLE
CHILD
YEARS
FAMILIES
WORK
PARENTS
SAYS
FAMILY
WELFARE
MEN
PERCENT
CARE
LIFE

SCHOOL
STUDENTS
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5:       label the input  $\mathbf{x}_i$  as belonging to the nearest cluster,
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$$y_i := \arg \min_{j=1, \dots, k} \|\mathbf{x}_i - \mathbf{c}_j\|^2$$

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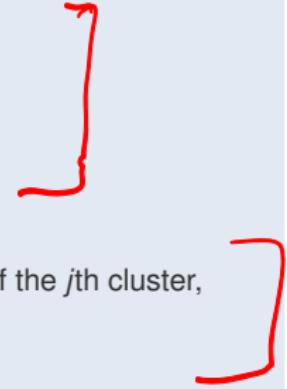
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11:    return cluster centers  $\mathbf{c}_1, \dots, \mathbf{c}_k$ 
12: end function
```



Demos

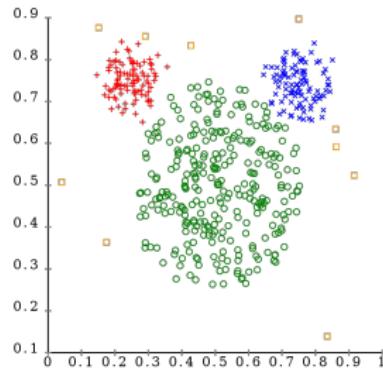
- ▶ http://home.deib.polimi.it/matteucc/Clustering/tutorial_html/AppletKM.html
- ▶ <http://www.cs.washington.edu/research/imagedatabase/demo/kmcluster/>
- ▶ <http://syskall.com/kmeans.js/>

Limitations:

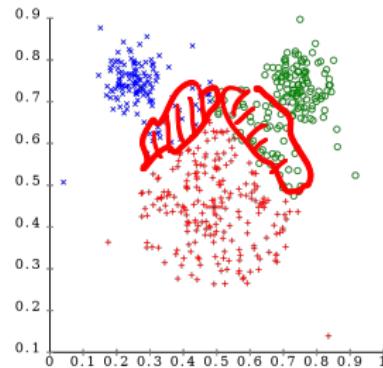
k-means Can Fail to Find the Right Clusters

Different cluster analysis results on "mouse" data set:

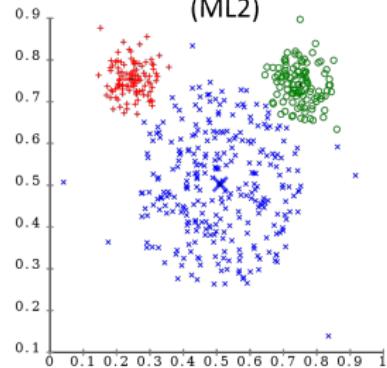
Original Data



k-Means Clustering



mixture of Gaussians
(ML2)



Will learn about an improvement of *k*-means in ML2: **mixture of Gaussians**

Limitations:

k-means Finds Linear Cluster Boundaries

Easiest to see for $k = 2$ clusters:

- ▶ Then the cluster boundary is the one of the nearest centroid classifier



Limitations:

k-means Finds Linear Cluster Boundaries

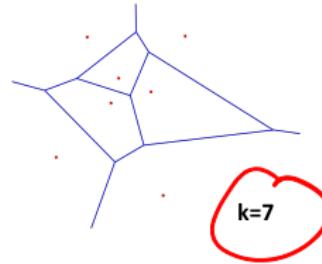
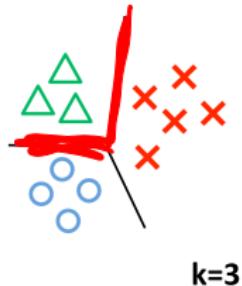
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- ▶ Then the cluster boundary is the one of the nearest centroid classifier



For $k \geq 3$ clusters:

- ▶ Cluster boundaries given by Voronoi diagram of cluster centers
- ▶ Thus the boundaries are (piecewise) linear



What to Do If the Ideal Decision Boundary is Non-linear?

