TECHNISCHE UNIVERSITÄT
KAISERSLAUTERN

9.1 Linear Clustering

Machine Learning 1: Foundations

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Recap

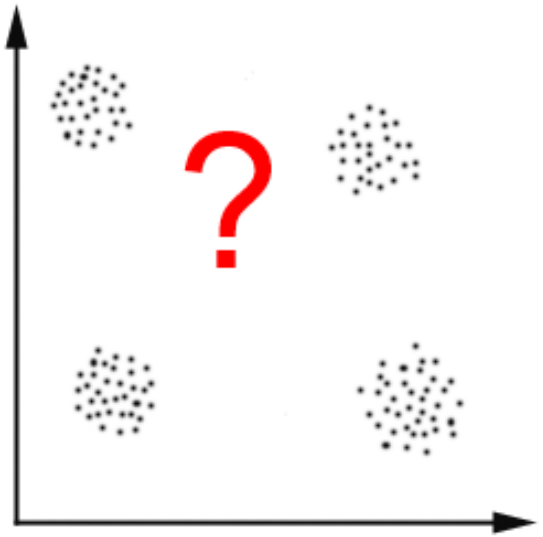
So far we have required so far in this course that both is given:

1. inputs $x_1, \ldots, x_n \in \mathbb{R}^d$
2. labels $y_1, \ldots, y_n$
   - with either $y_i \in \{-1, +1\}$ (for binary classification)
   - or $y_i \in \mathbb{R}$ (for regression)

This learning setting is called **supervised learning**.

But what if there are no labels given?

This setting is called **unsupervised learning**.



Today and Next Week

Definition

Unsupervised learning is the area of machine learning where

- we are given inputs $x_1, \ldots, x_n \in \mathbb{R}^d$
- but **no label**s $y_1, \ldots, y_n$.

What could be interesting tasks in unsupervised learning?

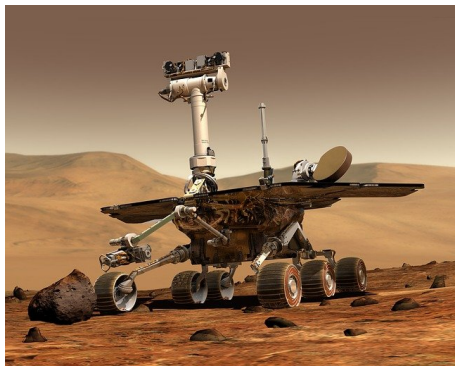
1. Anomaly Detection

Detect unusual data points

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

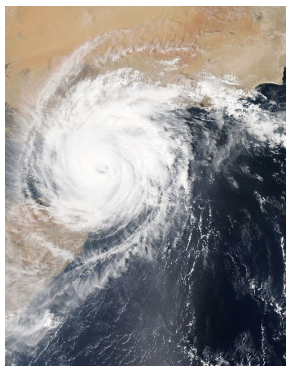
Examples:

Corrupt data



Novelties

Outliers

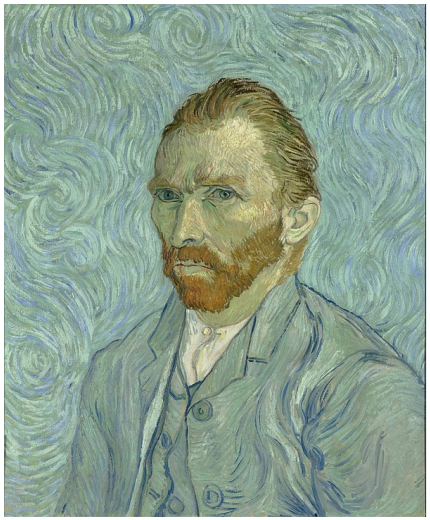
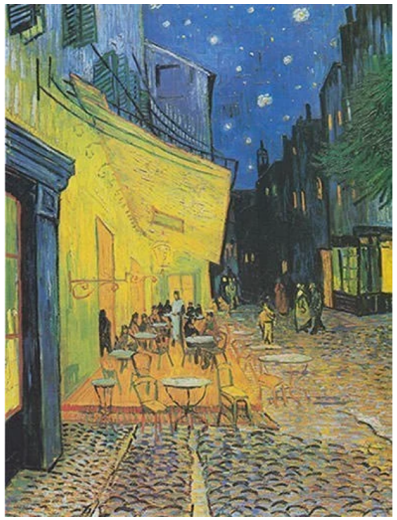
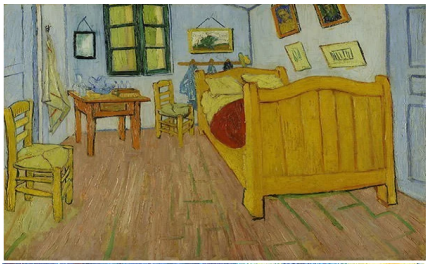


Rare events

Attacks on networks

2. Density Estimation and Generative Models

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


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

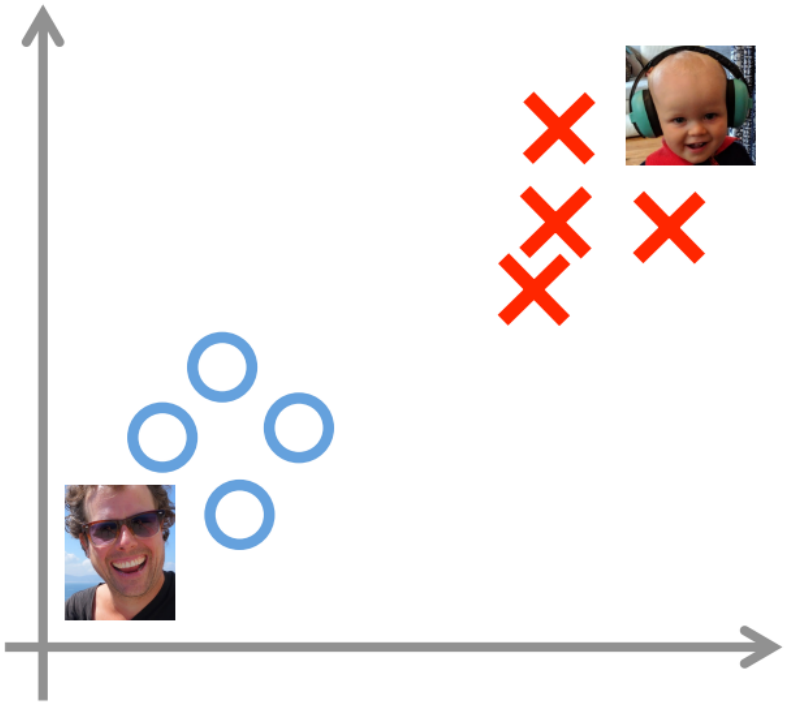

We will learn in **ML2** how this works

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

Compress data into lower-dimensional representation

Applications:

- data visualization
- data de-noising



4. Clustering

Today!

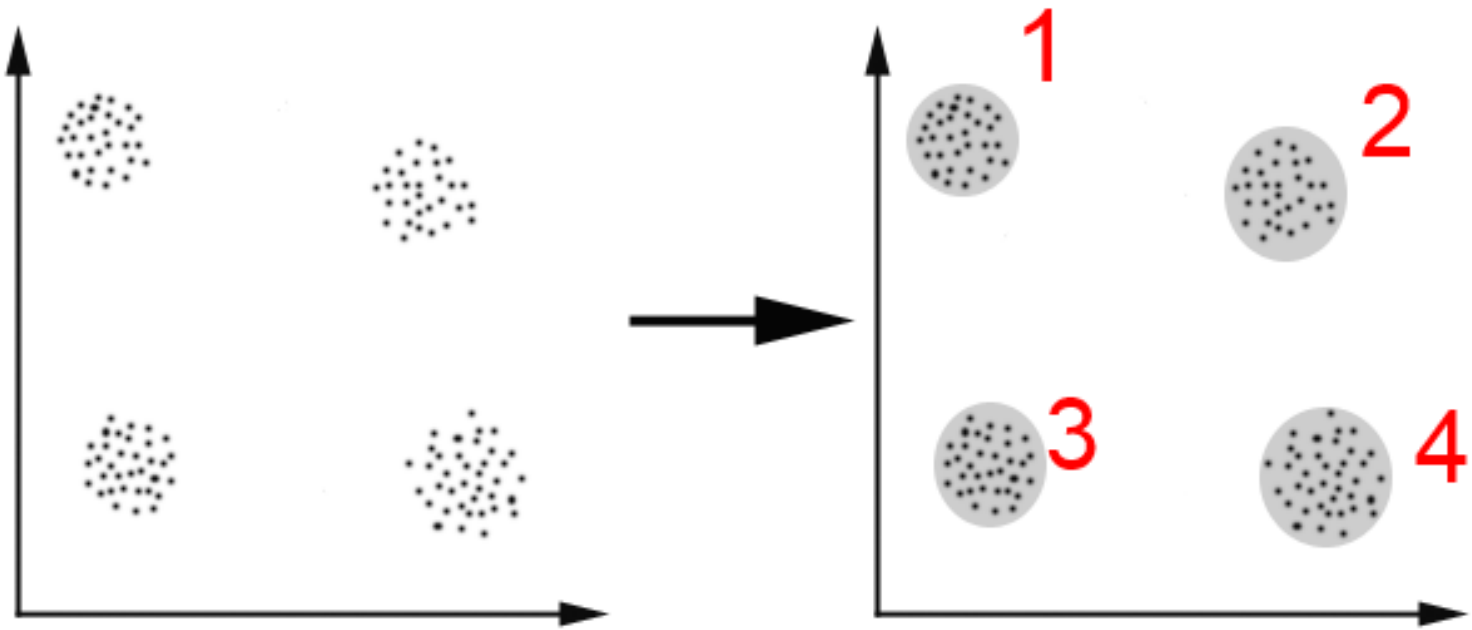
Contents of this Class

Clustering

What is Clustering?

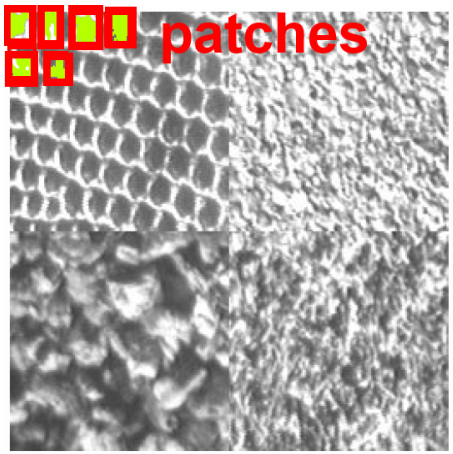
Definition

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



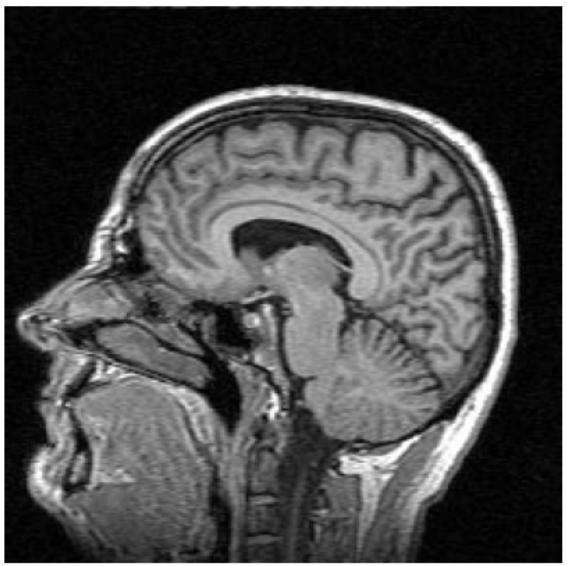
Example: Image Segmentation

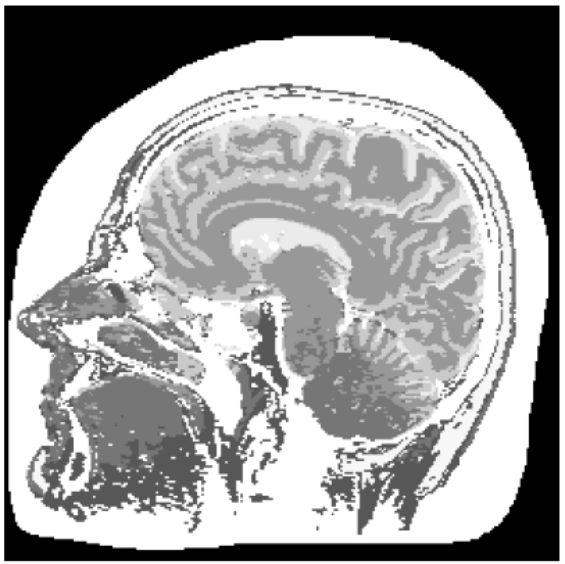
Original image:



each patch is a training example

segmented image





More examples

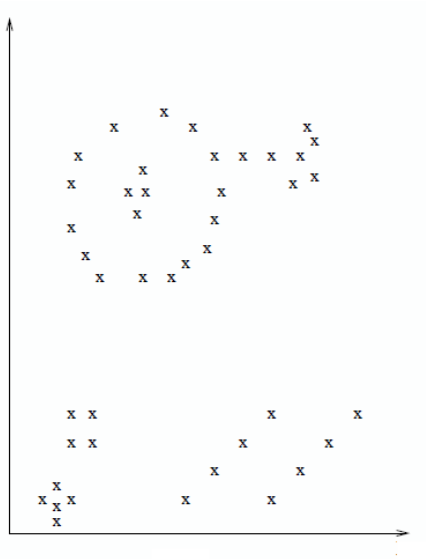
- **Recommender systems**: organizing products and customers into groups that are similar
- **Social networks**: cluster users into groups that have similar interests/preferences
- **WWW document classification**: organize webpages (e.g., news articles) into clusters with similar content (sports, ecnomonics, ...)

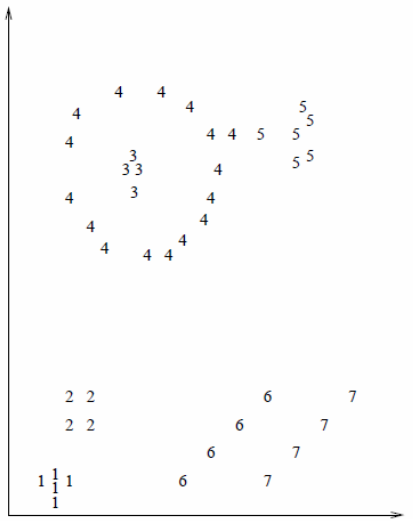
Clustering Dilemna

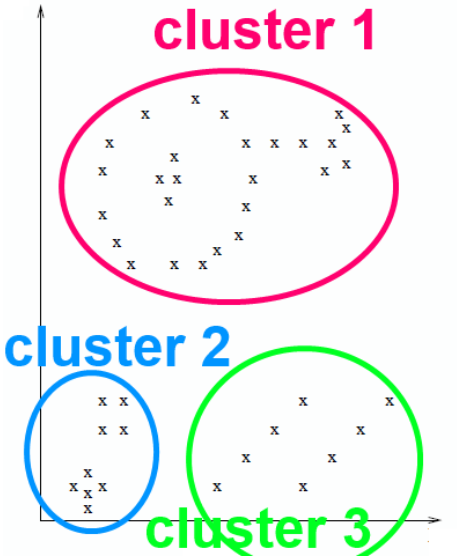
Big problem:

- evaluation of results!

Why? Quiz: how many clusters in this example?







7 clusters vs. 3 clusters

Evaluation of results

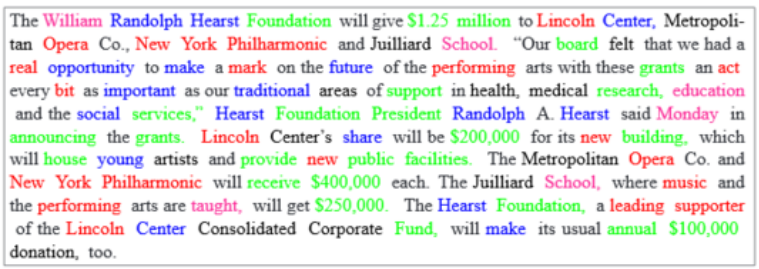
- Ground truth unknown **(no labels!)**

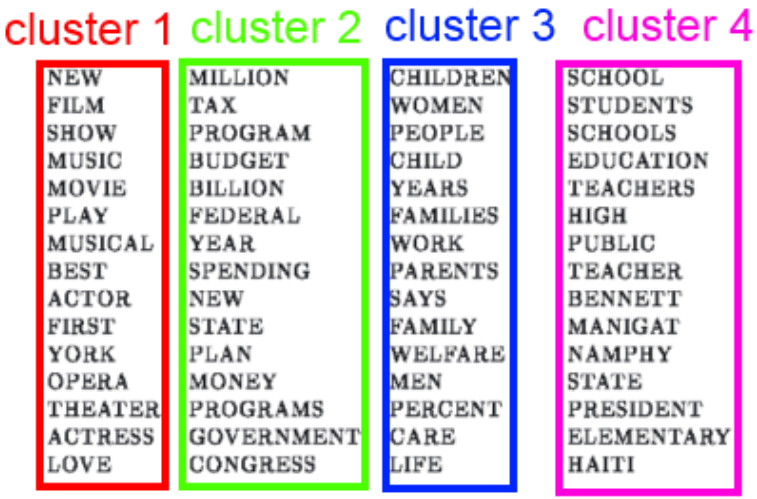
$\Rightarrow$ Results need to be inspected manually

- Example:
  - Given collection of documents,

The William Randolph Hearst Foundation will give $1.25 million to Lincoln Center, Metropolitan Opera Co., New York Philharmonic and Juilliard School. "Our board felt that we had a real opportunity to make a mark on the future of the performing arts with these grants an act every bit as important as our traditional areas of support in health, medical research, education and the social services," Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center's share will be $200,000 for its new building, which will house young artists and provide new public facilities. The Metropolitan Opera Co. and New York Philharmonic will receive $400,000 each. The Juilliard School, where music and the performing arts are taught, will get $250,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual $100,000 donation, too.

  - cluster words into groups





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  - cluster words into groups **& manual labeling**

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Arts	Budgets	Child	Education
NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
MUSIC	BUDGET	CHILD	EDUCATION
MOVIE	BILLION	YEARS	TEACHERS
PLAY	FEDERAL	FAMILIES	HIGH
MUSICAL	YEAR	WORK	PUBLIC
BEST	SPENDING	PARENTS	TEACHER
ACTOR	NEW	SAYS	BENNETT
FIRST	STATE	FAMILY	MANIGAT
YORK	PLAN	WELFARE	NAMPHY
OPERA	MONEY	MEN	STATE
THEATER	PROGRAMS	PERCENT	PRESIDENT
ACTRESS	GOVERNMENT	CARE	ELEMENTARY
LOVE	CONGRESS	LIFE	HAITI

k-means Clustering Algorithm

Arguably the most popular clustering algorithm is the following:

function KMEANS(parameter k, inputs $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$)
  initialize cluster centers $\mathbf{c}_1, \ldots, \mathbf{c}_k$
  (e.g., randomly drawn inputs $\mathbf{c}_j := \mathbf{x}_{i_j}$)
  repeat
    for $i = 1 : n$ **do**
      label the input $\mathbf{x}_i$ as belonging to the nearest cluster,

$$y_i := \operatorname*{arg\,min}_{j=1,\ldots,k} \left\| \mathbf{x}_i - \mathbf{c}_j \right\|^2$$

    end for
    for $j = 1 : k$ **do**
      compute cluster center $\mathbf{c}_j$ as the mean of all inputs of the jth cluster,

$$\mathbf{c}_j := \operatorname{mean}(\{\mathbf{x}_i : y_i = j\})$$

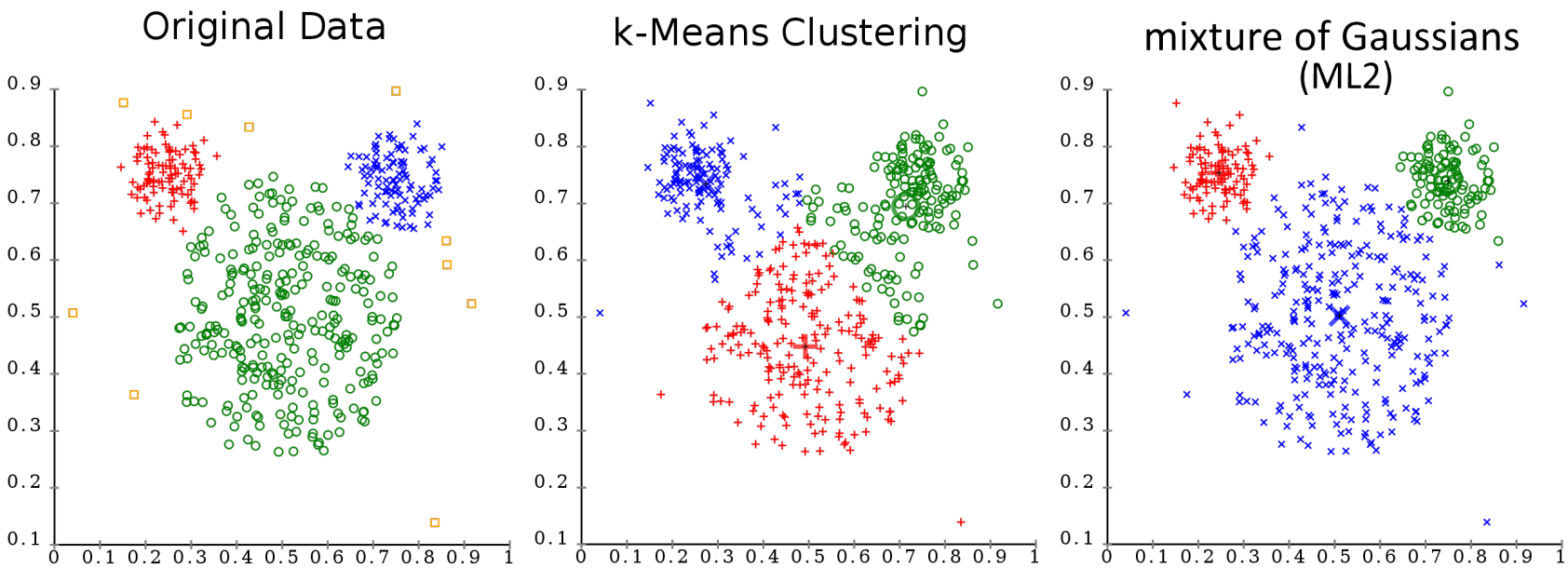
    end for
  until convergence criterion is met
  (e.g., no change in clusters between subsequent iterations)
  return cluster centers $c_1, \ldots, c_k$
end function

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: 1/2
k-means Can Fail to Find the Right Clusters

Different cluster analysis results on "mouse" data set:



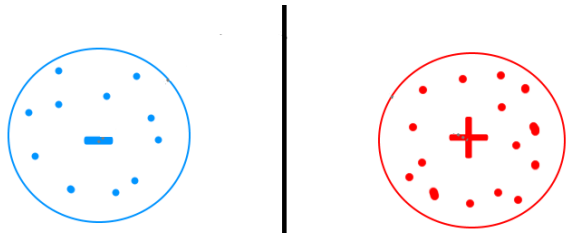
Will learn about an improvement of *k*-means in ML2: **mixture of Gaussians**

Limitations:

k-means Finds **Linear** Cluster Boundaries

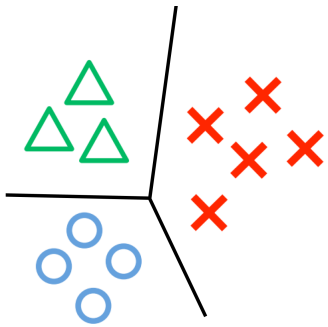
Easiest to see for $k = 2$ clusters:

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

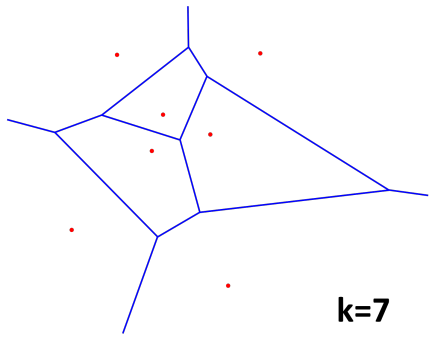


For $k \geq 3$ clusters:

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



k=3



k=7

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