

# IB031 Úvod do strojového učení

Tomáš Brázdil

# Course Info

## Resources:

- ▶ Lectures & tutorials (the **main** source)
- ▶ Many books, few perfect for introductory level  
One relatively good, especially the first part:  
A. Géron. Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems. O'Reilly Media; 3rd edition, 2022
- ▶ (Almost) infinitely many online courses, tutorials, materials, etc.

# Evaluation

The evaluation is composed of three parts:

- ▶ Mid-term exam: Written exam from the material of the first half of the semester.
- ▶ End-term exam: The "big" one containing everything from the semester (with possibly more stress in the second half).
- ▶ Projects: During tutorials, you will work on larger projects (in pairs or triples).

Each part contributes the following number of points:

- ▶ Mid-term exam: 25
- ▶ End-term exam: 50
- ▶ Project: 25

To pass, you need to obtain at least 60 points.

# Distinguishing Properties of the Course

- ▶ Introductory, prerequisites are held to a minimum
- ▶ Formal and precise: Be prepared for a complete and “mathematical” description of presented methods.



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I assume that you have basic knowledge of

- ▶ Elementary mathematical notation (operations on sets, logic, etc.)
- ▶ Linear algebra: Vectors in  $\mathbb{R}^n$ , operations on vectors (including the dot product). Geometric interpretation!
- ▶ Calculus: Functions of multiple real variables, partial derivatives, basic differential calculus.
- ▶ Probability: Notion of probability distribution, random variables/vectors, expectation.

# What Is Machine Learning?

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Here is a slightly more general definition:

**Arthur Samuel, 1959**

Machine learning is the field of study that allows computers to learn without being explicitly programmed.

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And a more engineering-oriented one:

Tom Mitchell, 1997

A computer program is said to learn from experience  $E$  concerning some task  $T$  and some performance measure  $P$  if its performance on  $T$ , as measured by  $P$ , improves with experience  $E$ .

## Example

In the context of spam filtering:

- ▶ The task  $T$  is to flag spam in new emails.
- ▶ The experience  $E$  is represented by a set of emails labeled either spam or ham by hand (the training data).
- ▶ The performance measure  $P$  could be the accuracy, which is the ratio of the number of correctly classified emails and all emails.

There are many more performance measures; we will study the basic ones later.

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In the context of housing price prediction:

- ▶ The task  $T$  is to predict prices of new houses based on their basic parameters (size, number of bathrooms, etc.)
- ▶ The experience  $E$  is represented by information about existing houses.
- ▶ The performance measure  $P$  could be, e.g., an absolute difference between the predicted and the real price.

## Examples (cont.)

In the context of game playing:

- ▶ The task  $T$  is to play chess.
- ▶ The experience  $E$  is represented by a series of self-plays where the computer plays against itself.
- ▶ The performance measure  $P$  is winning/losing the game.

Here, the trick is to spread the delayed and limited feedback about the result of the game throughout the individual decisions in the game.

## Examples (cont.)

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In the context of customer behavior:

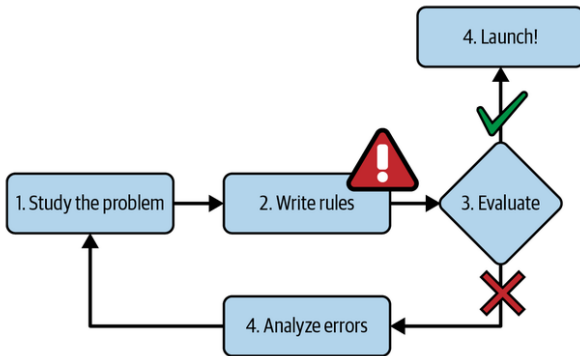
- ▶ The task  $T$  is to group customers with similar shopping habits in an e-shop.
- ▶ The experience  $E$  consists of lists of items individual customers bought in the shop.
- ▶ The performance measure  $P$ ?  
Measure how "nicely" the customers are grouped.  
(whether people with similar habits, as seen by humans, fall into the same group).



# Comparison of Programming and Learning

How to code the spam filter?

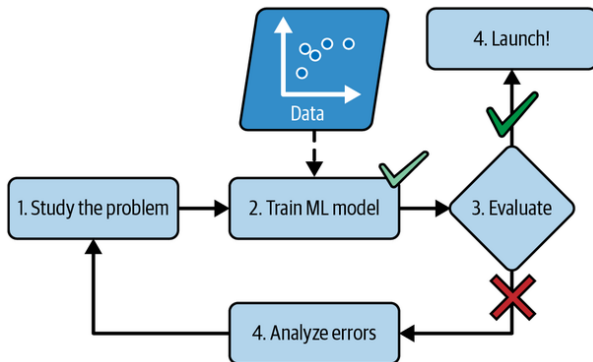
- ▶ Examine what spam mails typically contain: Specific words ("Viagra"), sender's address, etc.
- ▶ Write down a rule-based system that detects specific features.
- ▶ Test the program on new emails and (most probably) go back to look for more spam features.



# Comparison of Programming and Learning

The machine learning way:

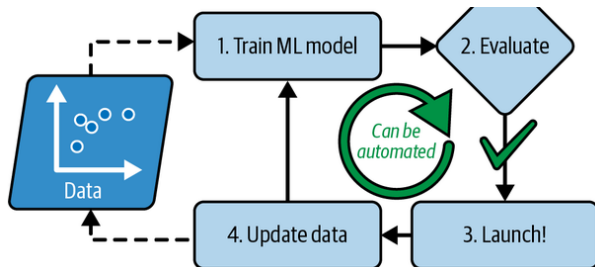
- ▶ Study the problem and collect lots of emails, labeling them spam or ham.
- ▶ Train a machine learning model that reads an email and decides whether it's spam or ham.
- ▶ Test the model and (most probably) go back to collect more data and adjust the model.



# ML Solutions are Adaptive

Spam filter: Authors of spam might and will adapt to your spam filter (possibly change the wording to pass through).

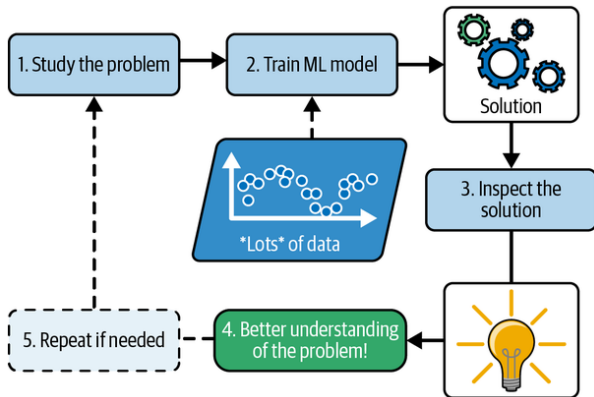
ML systems can be adjusted to new situations by retraining on new data (unless the data becomes ugly).



# ML for Human Understanding

Spam filter: A trained system can be inspected for notorious spam features.

Some models allow direct inspection, such as decision trees or linear/logistic regression models.



# Usage of Machine Learning

Machine learning suits various applications, especially where traditional methods fall short. Here are some areas where it excels:

- ▶ Solving complex problems where fine-tuning and rule-based solutions are inadequate.
- ▶ Tackling complex issues that resist traditional problem-solving approaches.
- ▶ Adapting to fluctuating environments through retraining on new data.
- ▶ Gaining insights from large and complex datasets.

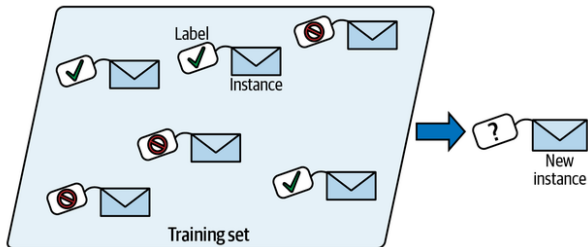
In summary, machine learning offers innovative solutions and adaptability for today's complex and ever-changing problems, (sometimes) providing insights beyond the reach of traditional approaches.

# Types of Learning

There are main categories based on information available during the training:

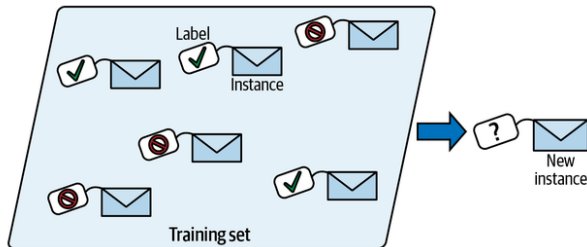
- ▶ Supervised learning
- ▶ Unsupervised learning
- ▶ Semi-supervised learning
- ▶ Self-supervised learning
- ▶ Reinforcement learning

# Supervised Learning



Labels are available for all input data.

# Supervised Learning



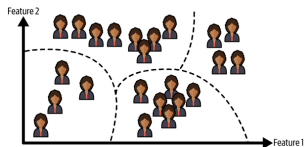
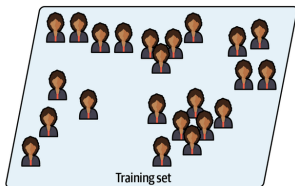
Labels are available for all input data.

Typical supervised learning tasks are

- ▶ *Classification* where the aim is to classify inputs into (typically few) classes  
(e.g., the spam filter where the classes are spam/ham)
- ▶ *Regression* where a numerical value is output for a given input  
(e.g., housing prices)

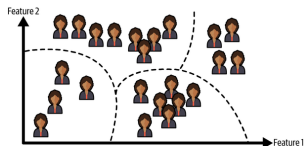
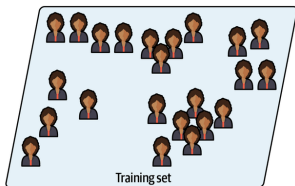


# Unsupervised Learning



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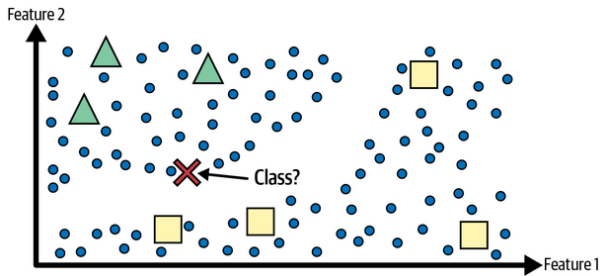


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Typical unsupervised learning tasks are

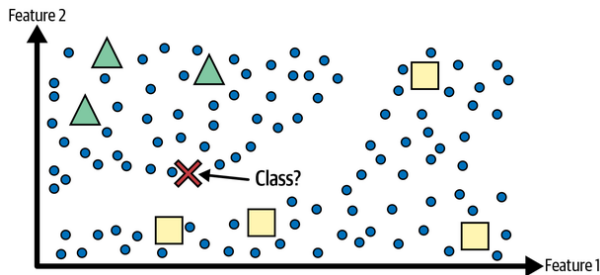
- ▶ *Clustering* where inputs are grouped according to their features  
(e.g., clients of a bank grouped according to their age, wealth, etc.)
- ▶ *Association* where interesting relations and rules are discovered among the features of inputs  
(e.g., market basket mining where associations between various types of goods are being learned from the behavior of customers)
- ▶ *Dimensionality reduction* reduce high-dimensional data to few dimensions (e.g., images to few image features)

# Semi-Supervised Learning



Labels for some data.

# Semi-Supervised Learning

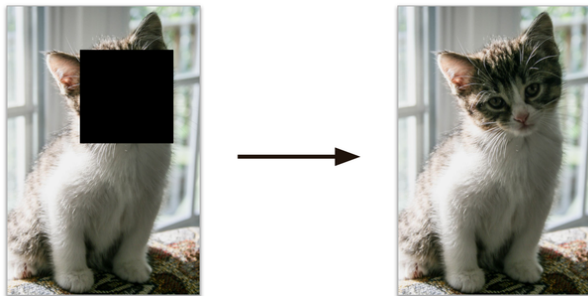


Labels for some data.

For example, Medical data, where elaborate diagnosis is available only for some patients.

Combines supervised and unsupervised learning: e.g., clusters all data and labels the unlabeled inputs with the most common labels in their clusters.

# Self-Supervised Learning

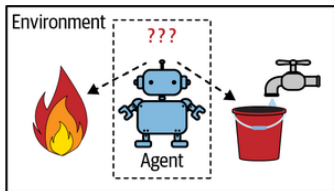


Generate labels from (unlabeled) inputs.

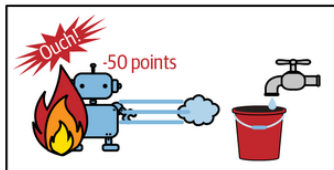
The goal is to learn typical features of the data.

It can be later modified to generate images, classify, etc.

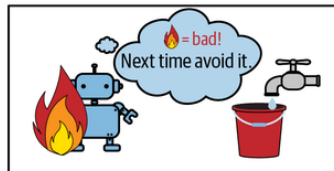
# Reinforcement Learning



- 1 Observe
- 2 Select action using policy



- 3 Action!
- 4 Get reward or penalty



- 5 Update policy (learning step)
- 6 Iterate until an optimal policy is found

Learn from performing *actions* and getting feedback from *environment*.

# ML Applications Highlights

- ▶ ChatGPT (and similar generative models)
  - ▶ The basis forms a generative language model, i.e., a text-generating model trained on texts in a self-supervised way
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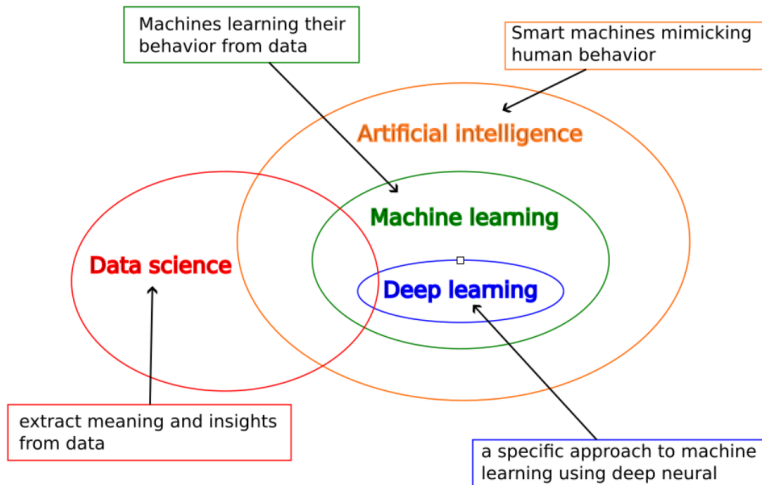
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  - ▶ Essential but not fancy
- ▶ Game playing: More fancy than useful, learning models beating humans in several difficult games.

# ML in Context



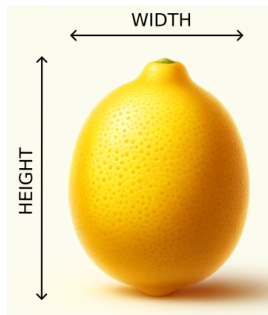
# Supervised Learning

## Example - Fruit Recognition

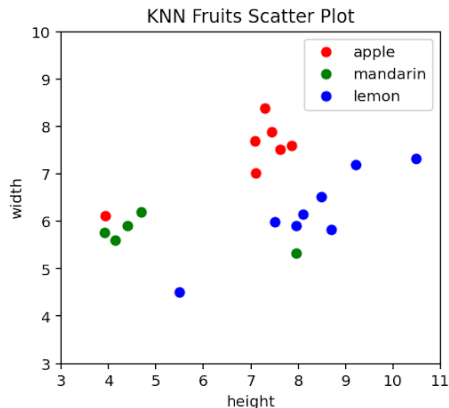
**The goal:** Create an automatic system for fruit recognition, concretely apple, lemon, and mandarin.

**Inputs:** Measures of *height* and *width* of each fruit.

Suppose we have a dataset of dimensions of several fruits labeled with the correct class.



# Data



	height	width	fruit
0	3.91	5.76	Mandarin
1	7.09	7.69	Apple
2	10.48	7.32	Lemon
3	9.21	7.20	Lemon
4	7.95	5.90	Lemon
5	7.62	7.51	Apple
6	7.95	5.32	Mandarin
7	4.69	6.19	Mandarin
8	7.50	5.99	Lemon
9	7.11	7.02	Apple
10	4.15	5.60	Mandarin
11	7.29	8.38	Apple
12	8.49	6.52	Lemon
13	7.44	7.89	Apple
14	7.86	7.60	Apple
15	3.93	6.12	Apple
16	4.40	5.90	Mandarin
17	5.50	4.50	Lemon
18	8.10	6.15	Lemon
19	8.69	5.82	Lemon

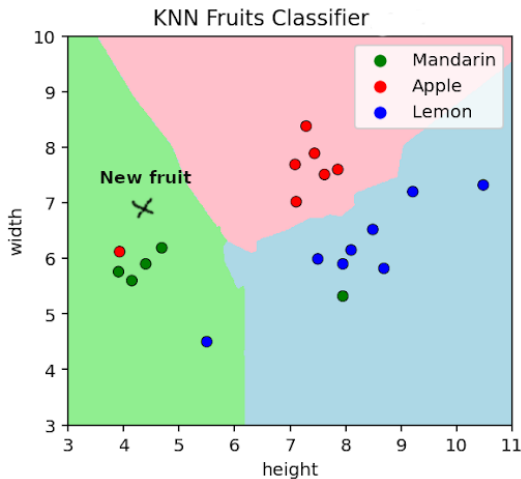
Use similarity to solve the problem.



# KNN Classification

Given a new fruit.  
What is it?

Find five closest  
examples



Where is the machine learning?

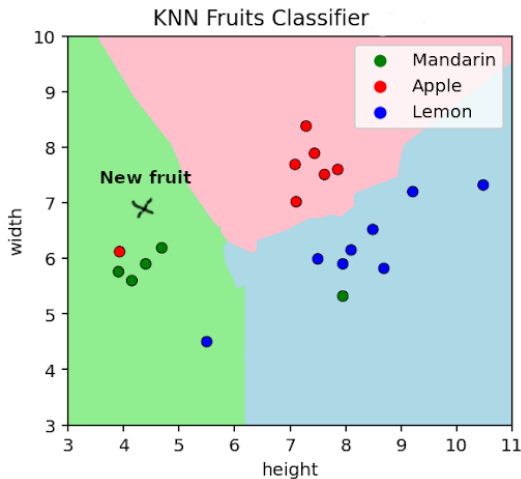
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Among the five closest:

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- ▶  $A = 1$  apples
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# KNN Classification

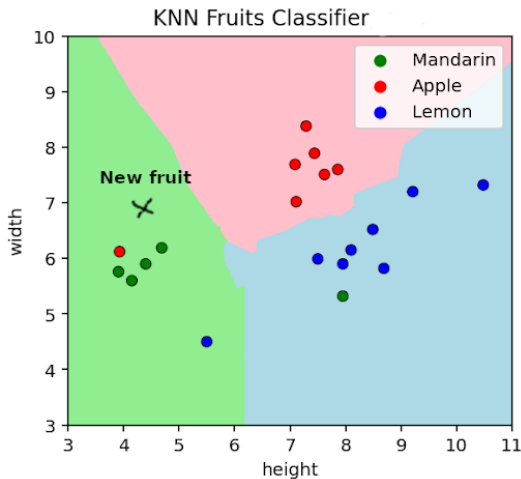
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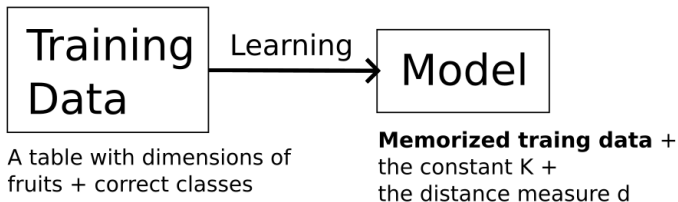
It is a **mandarin**!



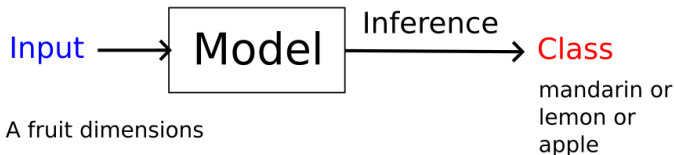
Where is the machine learning?

# Learning in Fruit Classification with KNN

**Learning:**



**Inference:**



# Fruit Classification Algorithm

**Input:** A fruit  $F$  with dimensions *height*, *width*

**Output:** *mandarin*, *lemon*, *apple*

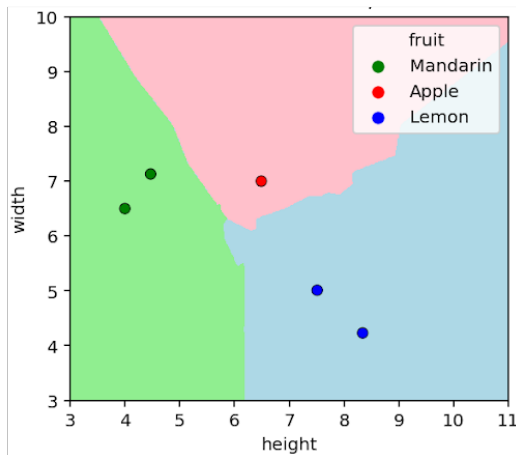
- 1: Find  $K$  examples  $\{E_1, \dots, E_K\}$  in the dataset whose dimensions are closest to the dimensions of the fruit  $F$
- 2: Count the number of examples of each class in  $\{E_1, \dots, E_K\}$ 
  - $M$  mandarins in  $\{E_1, \dots, E_K\}$
  - $L$  lemons in  $\{E_1, \dots, E_K\}$
  - $A$  apples in  $\{E_1, \dots, E_K\}$
- 3: **if**  $M \geq L$  and  $M \geq A$  **then return** *mandarin*
- 4: **else if**  $L \geq A$  **then return** *lemon*
- 5: **else return** *apple*
- 6: **end if**

Does it work?

# Testing the Model for Fruit Classification

Consider a test set of new instances ( $K = 5$ ,  $d$  is Euclidean):

height	width	fruit
4.0	6.5	Mandarin
4.47	7.13	Mandarin
6.49	7.0	Apple
7.51	5.01	Lemon
8.34	4.23	Lemon



Perfect classification of new data! Just deploy and sell!!

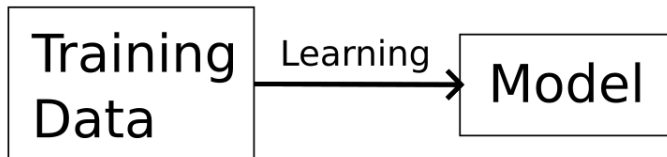
# K Nearest Neighbors

... on ideal data

# Learning and Inference

Two crucial components of machine learning are the following:

**Learning:**  
Creating model



**Inference:**  
Using model





# Training Data

Assume table training data, i.e., of the form

$x_{11}$	$x_{12}$	$\cdots$	$x_{1n}$	$c_1$
$x_{21}$	$x_{22}$	$\cdots$	$x_{2n}$	$c_2$
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$x_{p1}$	$x_{p2}$	$\cdots$	$x_{pn}$	$c_p$

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Formally, we define **training dataset**

$$\mathcal{T} = \{(\vec{x}_k, c_k) \mid k = 1, \dots, p\}$$

Here each  $\vec{x}_k \in \mathbb{R}^n$  is an input vector and  $c_k \in C$  is the correct class.

$$\mathcal{T} = \{(4.0, 6.5), M), \\ (4.47, 7.13), M), \\ (6.49, 7.0), A), \\ \dots\}$$

# KNN: Learning

Consider the training set:

$$\mathcal{T} = \{(\vec{x}_k, c_k) \mid k = 1, \dots, p\}$$

and *memorize it* exactly as it is.

Store in a table.

Possibly use a clever representation allowing fast computation of nearest neighbors such as KDTrees (out of the scope of this lecture).

Also,

- ▶ determine the number of neighbors  $K \in \mathbb{N}$ ,
- ▶ and the distance measure  $d$ .

## Inference in KNN

Assume a KNN "trained" by memorizing

$\mathcal{T} = \{(\vec{x}_k, c_k) \in \mathbb{R}^n \times C \mid k = 1, \dots, p\}$ , a constant  $K \in \mathbb{N}$  and a distance measure  $d$ .

For  $d$ , consider Euclidean distance, but different norms may also be used to define different distance measures.

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**Input:** A vector  $\vec{z} = (z_1, \dots, z_n) \in \mathbb{R}^n$

**Output:** A class from  $C$

- 1: Find  $K$  indices of examples  $X = \{i_1, \dots, i_K\} \subseteq \{1, \dots, p\}$  with minimum distance to  $\vec{z}$ , i.e., satisfying

$$\max\{d(\vec{z}, \vec{x}_\ell) \mid \ell \in X\} \leq \min\{d(\vec{z}, \vec{x}_\ell) \mid \ell \in \{1, \dots, p\} \setminus X\}$$

- 2: For every  $c \in C$  count the number  $\#c$  of elements  $\ell$  in  $X$  such that  $c_\ell = c$
- 3: Return some

$$c_{\max} \in \arg \max_{c \in C} \#c$$

A class  $c_{\max} \in C$  which maximizes  $\#c$ .

# The resulting model

What exactly constitutes the model? The *model* consists of

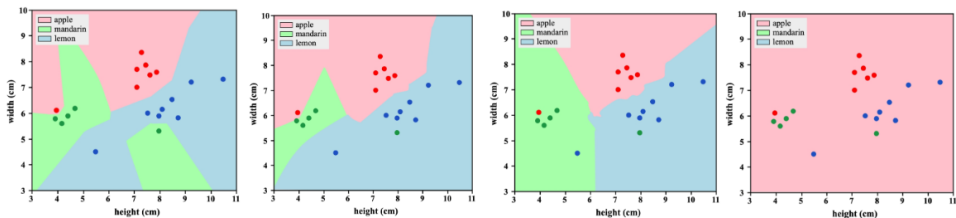
- ▶ The *trained parameters*: In this case the memorized training data.
- ▶ The *hyperparameters* set “from the outside”: In this case, the number of neighbors  $K$  and the distance measure  $d$ .

# The resulting model

What exactly constitutes the model? The *model* consists of

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Note that different settings of  $K$  lead to different classifiers (for the same  $d$ ):



## In Practice

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- ▶ Deal with issues in the data
  - ▶ Data almost always comes in weird formats, with inconsistencies, missing values, wrong values, etc.
  - ▶ Data rarely have the ideal form for a given learning model.

We need to ingest, validate, and preprocess the data.



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- ▶ Deal with the wrong model by testing and validation in as realistic conditions as possible.

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  - ▶ Data rarely have the ideal form for a given learning model.

We need to ingest, validate, and preprocess the data.

- ▶ Deal with issues in the model
  - ▶ In KNN, the training memorizes the example, but at least the  $K$  can be tuned.

We need to tune the model.

- ▶ Deal with the wrong model by testing and validation in as realistic conditions as possible.
- ▶ Deal with deployment - real-world application issues involving, e.g., implementation in embedded devices with limited resources.

# Models Considered in This Course

Throughout this course, we will meet the following models:

- ▶ KNN (already did)
- ▶ Decision trees
- ▶ (Naive) Bayes classifier
- ▶ Clustering: K-means and hierarchical
- ▶ Linear and logistic regression
- ▶ Support Vector Machines (SVM)
- ▶ Kernel linear models
- ▶ Neural networks (light intro to feed-forward networks)
- ▶ Ensemble methods + random forests
- ▶ (maybe some reinforcement learning)

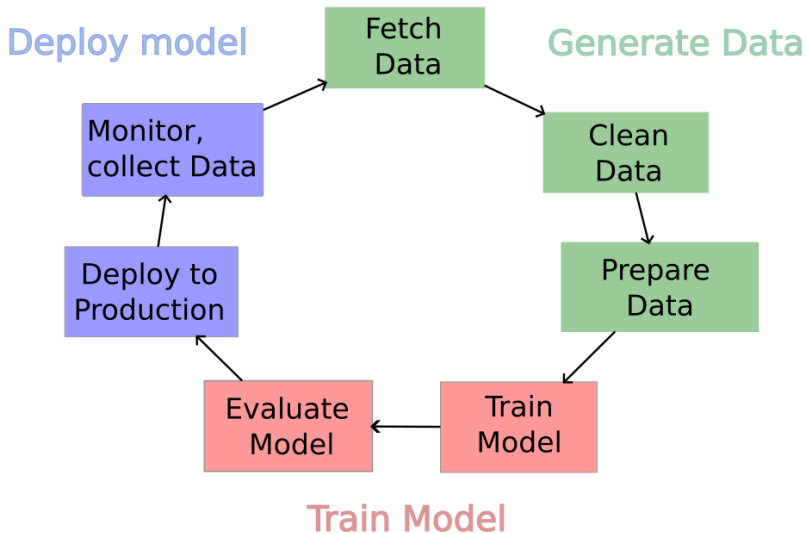
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...but first, let us see the whole machine-learning pipeline.

# Machine Learning Pipeline



# Fetch Data

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- ▶ Integrate data from various sources.

A serious diagnostic system must be trained/tested on data from many hospitals. You must blend the data from various sources (different formats, etc.).

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At this point, you should randomize the ordering of the data and select a test set to be used in model evaluation!

The test data are supposed to simulate the actual conditions, i.e., they should be “unseen”.

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## **Data Exploration**

Compute basic statistics to identify missing values, outliers, etc.

# Clean Data

The cleaning usually comprises the following steps:

- ▶ Fix or remove incorrect or corrupted values.
- ▶ Identify outliers and decide what to do with them.  
Outliers may harm some training methods and are not “representative”. However, sometimes, they naturally belong to the dataset, and expert insight is needed.
- ▶ Fix formatting.  
For example, the Date may be expressed in many ways, and a simple Yes/No answer.
- ▶ Resolve missing values (by either removing the whole examples or imputing)  
Many methods have been developed for missing values imputation. It is a susceptible issue because new values may strongly bias the model.
- ▶ Remove duplicates.

The above steps often affect the training and need expertise in the application domain.

Later in this course, we will discuss techniques for data cleaning.



ID	Age	Income	Gender	Customer_Satisfaction
1	38	46641.356413713	nan	Unsatisfied
2	42	49129.0615585107	female	Neutral
3	18	119965.049731014	Male	nan
4	18	66828.0762224329	nan	very unsatisfied
5	58	57422.2721106762	female	very unsatisfied
6	28	59502.8174855665	Other	Satisfied
7	18	42659.6675768587	Other	Neutral
8	18	54019.1173206374	Other	Satisfied
9	40	25429.1604541137	female	Unsatisfied
10	21	15595.5862129548	Other	Satisfied
11	18	58094.2328460069	Other	very unsatisfied
12	18	39097.3278583155	female	Very Satisfied
13	30		Other	Satisfied
14	50	30617.3914472273	Female	Very Satisfied
15	18		nan	Neutral
16	34	39902.4430953214	male	nan
17	49	68381.6997683133	Female	Very Satisfied
18	33	44796.0962271524	Other	Very Satisfied
19	47	39218.9560738814	Female	very unsatisfied
20		14544.9226784447	Other	Satisfied

# Prepare Data

Unlike cleaning, which is application-dependent, data preparation/transformation is model-dependent. This usually subsumes:

- ▶ **Scaling:** Settings values of inputs to a similar range.

Some models, especially those utilizing distance, are sensitive to large differences between input sizes.

- ▶ **Encoding:** Encode non-numeric data using real-valued vectors.

Many models, especially those based on geometry, work only with numeric data. Non-numeric data such as Yes/No, Short/Medium/Long must be encoded appropriately.

- ▶ **Binning or Discretization** Convert continuous features into discrete bins to capture patterns in ranges.

**Comment:** Sometimes **Normalization**, that is changing the distribution of inputs to resemble the normal distribution, is mentioned. However, this step is typically not essential for machine learning itself. However, it is important to use statistical inference to test the significance of learned parameters.

# Prepare Data

- ▶ **Feature selection** Throw out input features that are too “similar” to other features.

For example, if the temperature is measured both in Celsius and in Kelvin, keep one of them. The relationship can, of course, be a more complex (non-linear) correlation.

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- ▶ **Dimensionality reduction** Transforming data from  $\mathbb{R}^n$  to  $\mathbb{R}^m$  where  $m \ll n$ .

Growing dimension means growing difficulty of training for all models. Some models cease to work for high-dimensional data. The reduction typically searches for a few important characteristic features of inputs.

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- ▶ **Feature aggregation** Introducing new features using operations on the original ones.

We will see kernel transformations later in this course, allowing simple models to solve complex problems.

## Train Model

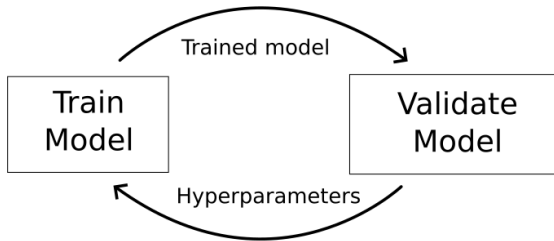
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# Train Model

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Before training, we should split the dataset into

- ▶ *training* dataset on which the model will learn
- ▶ *validation* dataset on which we fine-tune hyperparameters



The resulting model is obtained after several iterations of the above process.

# Evaluate Model

Here, we use the test set that we separated during data fetching.

In some cases, a brand new test set can be generated.

patients are examined regularly, creating new records continuously.

In some cases, it is tough to obtain new data.

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**Critical issue:** Make sure that you are truly testing  
exactly the whole inference process.

Often, just a model is tested, and the testing and production inference engines are separated. This leads to truly nasty errors in the production!

We will discuss various generic metrics helpful in measuring the quality of the resulting model.

## Deploy to Production

Deployment of machine learning models is a complex question, application dependent.

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From the technical point of view, the typical issues solved by ML Ops teams are

- ▶ how to extract/process data in real-time
- ▶ how much storage is required
- ▶ how to store/collect model (and data) artifacts/predictions
- ▶ how to set up APIs, tools, and software environments
- ▶ What the period of predictions (instantaneous or batch predictions) should be
- ▶ how to set up hardware requirements (or cloud requirements for on-cloud environments) by the computational resources required
- ▶ how to set up a pipeline for continuous training and parameter tuning

# Deploy to Production

From the user's point of view:

- ▶ How to get a sensible and valuable user output?
  - ▶ AI researchers will be satisfied with tons of running text in terminals.
  - ▶ “Normal” people need a graphical interface with understandable output.
  - ▶ Experts working in other domains typically demand speed and clarity at the extreme.

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  - ▶ “Normal” people need a graphical interface with understandable output.
  - ▶ Experts working in other domains typically demand speed and clarity at the extreme.
- ▶ How do you persuade users that the AI is working for them?
  - ▶ Especially if safety is at stake, you need to have outstanding arguments and explanations ready for end-users.
  - ▶ In many areas, the devices need to be certified (medicine, automotive) for ML-based systems.

This complex subject will be only touched on in this course.

## Monitor, collect Data

Deployed machine learning models must be constantly monitored.

Because of the influx of new data, ML models work in highly dynamic environments.

For example, an image-processing medical diagnostic model suddenly misdiagnosed a patient because a nurse marked the sample with a marker pen.

Every customer has a different infrastructure and may produce data slightly differently.

Data for retraining and improvement should be stored.

Also, many areas allow the *active learning* where users provide feedback for (continuous) retraining of the models.

Data

## Data Science Example

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The data consists of a 1000 lines table with five columns:

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The aim is to predict the last field given the others.

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After a few days, you have trained a model that predicts numbers resembling the ones in the table.

You contact the medical researcher and discuss the results.

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**Researcher:** Well, first, there is field 5, the variable we want to predict. It's common knowledge among people who analyze this type of data that results are better if you work with the log of the values, but I didn't discover this until later. Was it mentioned to you?



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**Data Miner:** No.

## Model Dicsuccion

**Researcher:** But surely you heard about what happened to field 4? It's supposed to be measured on a scale from 1 to 10, with 0 indicating a missing value, but because of a data entry error, all 10's were changed into 0's. Unfortunately, since some of the patients have missing values for this field, it's impossible to say whether a 0 in this field is a real 0 or a 10. Quite a few of the records have that problem.

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**Data Miner:** Yes, but these fields were only weak predictors of field 5.

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**Researcher:** Anyway, given all those problems, I'm surprised you were able to accomplish anything.

**Data Miner:** True, but my results are really quite good. Field 1 is a very strong predictor of field 5. I'm surprised that this wasn't noticed before.

**Researcher:** What? Field 1 is just an identification number.

**Data Miner:** Nonetheless, my results speak for themselves.

**Researcher:** Oh, no! I just remembered. We assigned ID numbers after we sorted the records based on field 5. There is a strong connection, but it isn't very sensible. Sorry.

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OK, what's the point?

You have to

Understand the task you want to solve and the data!

# Data Objects

*Data objects* represent entities we work with (e.g., classify them).

For example, in cancer prediction, the data objects are patients. In fruit classification, the data objects are individual fruits.



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Data objects are described by *attributes* (or *features* or *variables*).

For example, the age, weight, genetic profile, and other patient characteristics. Or the width and height of a fruit.

# Attributes vs Features vs Variables

The name differs from field to field.

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So, the following names are usually used as synonyms:

- ▶ *Attributes* - used mostly by database and data mining experts.
- ▶ *Features* - used mostly by machine learning experts.
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One may make some distinctions

- ▶ *Attributes* represent information about the object without any additional assumptions.
- ▶ *Features* assume that their values are somewhat characteristic of the object.
- ▶ *Variables* assume that there is some process behind them (typically a random process in the case of statistics).

# Data Types - Categorical Attributes

*Categorical attributes* (nominal attributes) are symbols or names of things.

- ▶ Each value represents some kind of category, code, or state.
- ▶ Values are not ordered and should not be used quantitatively (in computer science, the values are known as enumerations).

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- ▶ **Examples:**

$\text{hair\_color} \in \{\text{black, brown, blond, red, auburn, gray, white}\}$

$\text{marital\_status} \in \{\text{single, married, divorced, widowed}\}$

$\text{customer\_ID} \in \{0, 1, 2, \dots\}$

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*Binary attributes* are categorical attributes with only two values.

## DataTypes - Ordinal Attributes

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## Examples:

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It can also be obtained by discretizing numeric quantities into series of intervals.

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Categorical and ordinal attributes are called *qualitative* attributes.

Next, we look at numeric, i.e., *quantitative* attributes.

## Data Types - Numeric Attributes

*Numeric attributes* are quantities represented by numbers.

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Distinguish two types: *Interval-scale* and *ratio-scale*.

	INTERVAL SCALE	RATIO SCALE
Measurement interval	Equal intervals between consecutive points.	Equal intervals with the presence of a true zero.
Absolute zero	Lacks a true zero point.	Possesses a true zero point.
Statistical analysis	Limited to addition and subtraction	Allows for meaningful multiplication and division.
Meaningful ratios	Ratios are not meaningful due to the lack of zero.	Ratios are meaningful due to the presence of zero.
Examples	Celsius temperature (20 degrees not twice as hot as 10 degrees)	Height, duration, etc. (20 meters is twice as large as 10 meters)

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A finite or countably infinite range of values, i.e., integers may represent the values.

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- ▶ *Continuous*

A continuous range of values, an interval.

There are several more or less formal definitions of continuous attributes in the literature. For example:

- ▶ All non-discrete variables.
- ▶ Have an infinite number of values between any two values.
- ▶ Their values are measured (??).

Deeper characteristics of data (statistical properties, etc.) will be examined at tutorials.

# Decision Trees



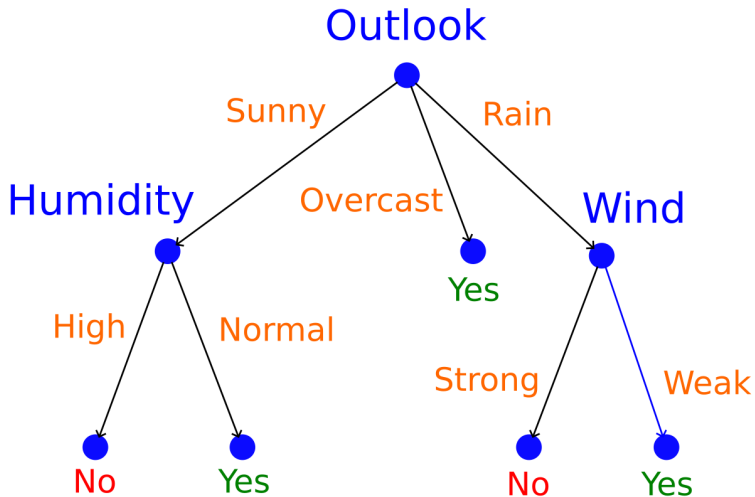
# Decision Trees

- ▶ One of the widely used methods for machine learning.
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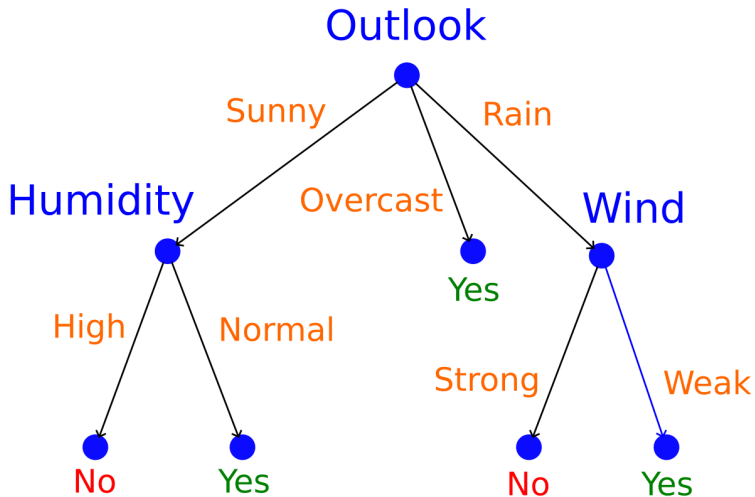
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- ▶ We will consider the ID3 algorithm.  
Quinlan, 1979
- ▶ Various adjustments that appear in C4.5, CART, etc.

Consider the weather forecast for tennis playing. How would you decide whether to play today?



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How do we obtain such a tree based on experience/data?

# Learning Decision Trees

Consider data represented as follows:

- ▶ A finite set of *attributes*  $\mathcal{A} = \{A_1, \dots, A_n\}$ .
- ▶ Each attribute  $A \in \mathcal{A}$  has its *set of values*  $V(A)$ .

We start with trees on discrete datasets, that is, assume  $V(A)$  finite for all  $A \in \mathcal{A}$ .

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Objects to be classified are described by vectors of values of all attributes:

$$\vec{x} = (x_1, \dots, x_n) \in V(A_1) \times \dots \times V(A_n)$$

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Consider a set  $C$  of *classes*.

We consider a multiclass classification in general, i.e.,  $C$  is an arbitrary finite set.

## Example

The tennis problem:

- ▶ The attributes are:

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- ▶  $C = \{\text{Yes}, \text{No}\}$

# Decision Trees

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A *decision tree* is

- ▶ a tree  $\mathcal{T} = (T, E)$  where
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- ▶ and there is a bijection between edges from  $\tau$  and values of the attribute  $A(\tau)$ . Given an edge  $(\tau, \tau') \in E$  we write  $V(\tau, \tau')$  to denote the value of the attribute  $A(\tau)$  assigned to the edge.

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**Inference:** Given an input  $\vec{x}$ , we traverse the tree from the root to a leaf, always choosing edges labeled with values of attributes from  $\vec{x}$ . The output is the class labeling the leaf.



## Example

$$T = \{O, H, W, z_1, z_2, z_3, z_4, z_5\}$$

$$T_{leaf} = \{z_1, z_2, z_3, z_4, z_5\}, T_{int} = \{O, H, W\}$$

$$E = \{(O, H), (O, W), (H, z_1), (H, z_2), \\ (O, z_3), (W, z_4), (W, z_5)\}$$

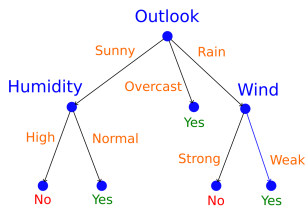
$$C(z_1) = C(z_4) = \text{No}, C(z_2) = C(z_3) = C(z_5) = \text{Yes}$$

$$A(O) = \text{Outlook}, A(H) = \text{Humidity}, A(W) = \text{Wind}$$

$$V(O, H) = \text{Sunny}, V(O, z_3) = \text{Overcast}, V(O, W) = \text{Rain}$$

$$V(H, z_1) = \text{High}, V(H, z_2) = \text{Normal}$$

$$V(W, z_4) = \text{Strong}, V(W, z_5) = \text{Weak}$$



**Inference:** For (*Rain, Hot, High, Strong*) we reach  $z_4$ , yielding *No*.

# Training Dataset

Consider a *training dataset*

$$\mathcal{D} = \{(\vec{x}_k, c_k) \mid k = 1, \dots, p\}$$

Here  $\vec{x}_k \in V(A_1) \times \dots \times V(A_k)$  and  $c_k \in C$  for every  $k$ .

Technically  $\mathcal{D}$  can be a multiset containing several occurrences of the same vector.

Index	Outlook	Temperature	Humidity	Wind	PlayTennis
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

$$\begin{aligned}
\mathcal{D} = \{ & ((Sunny, Hot, High, Weak), No), \\
& ((Sunny, Hot, High, Strong), No) \\
& \dots \\
& ((Rain, Mild, High, Strong), No) \}
\end{aligned}$$

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- ▶ Otherwise, identify an attribute  $A \in \mathcal{A}$  which *best classifies* the examples in  $\mathcal{D}$ . For every  $v \in V(A)$  we obtain

$$\mathcal{D}_v = \{\vec{x} \mid \vec{x} \in \mathcal{D}, A(\vec{x}) = v\}$$

We aim to have each  $\mathcal{D}_v$  as pure as possible, that is, ideally, to contain examples of just a single class.

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```
1: function ID3(dataset  $\mathcal{D}$ , attribute set  $\mathcal{A}$ )
2:   Create a root node  $\tau$  for the tree
3:   if  $\mathcal{D} = \emptyset$  then
4:     Return the single node  $\tau$  assigned with a default class.
5:   else if all examples in  $\mathcal{D}$  are of the same class  $c$  then
6:     Return the single-node tree, where  $\tau$  is assigned  $c$ 
7:   else if set of attributes  $\mathcal{A}$  is empty then
8:     Return the single-node tree where  $\tau$  is assigned
       the most common class in  $\mathcal{D}$ 
9:   else
10:    Choose attribute  $A \in \mathcal{A}$  best classifying examples in  $\mathcal{D}$ .
11:    Set the decision attribute for  $\tau$  to  $A$ 
12:    for each value  $v \in D(A)$  do
13:      Compute a decision tree  $\text{ID3}(\mathcal{D}_v, \mathcal{A} \setminus \{A\})$  with root  $\tau_v$ ,
14:      add a new edge  $(\tau, \tau_v)$  assigned  $v$ .
15:    end for
16:  end if
17: return  $\tau$ 
18: end function
```

# Best Classifying Attribute

We aim to choose an attribute that best informs us about the class.

As a result, we would possibly use as few attributes as possible and obtain a small tree containing only class-relevant decisions.

How to choose an attribute that best classifies examples in  $\mathcal{D}$ ?

There are several measures used in practice.

The most common are

- ▶ *information gain*
- ▶ *Gini impurity decrease*

## Information Gain

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We need some notation:

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$$Entropy(\mathcal{D}) = \sum_{c \in \mathcal{C}} -p_c \log_2 p_c$$

- ▶ The *information gain* of an attribute  $A$  is then defined by

$$Gain(\mathcal{D}, A) = Entropy(\mathcal{D}) - \sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Entropy(\mathcal{D}_v)$$

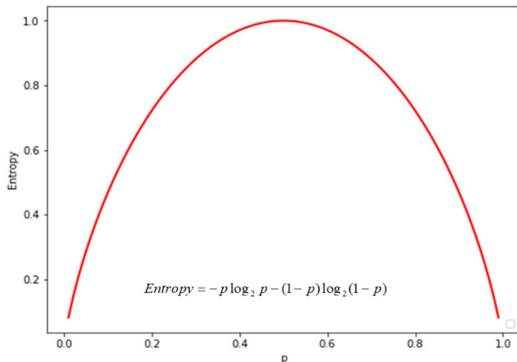
In every step of the ID3 algorithm, we choose an attribute *maximizing* the information gain for the current dataset  $\mathcal{D}$ .



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The intuition behind information gain:

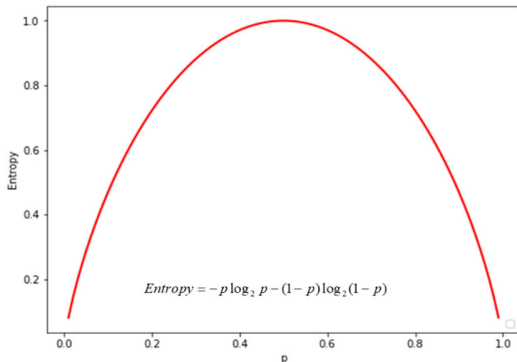
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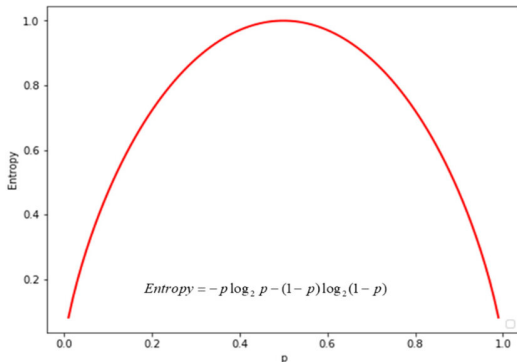


- $\sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Entropy(\mathcal{D}_v)$  is weighted uncertainty of classes in each  $\mathcal{D}_v$  (weighted by the relative size of  $\mathcal{D}_v$ ).

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- $Gain(\mathcal{D}, A)$  measures reduction in uncertainty of classes by splitting  $\mathcal{D}$  according to  $A$ .

# Gini Impurity

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- ▶ The *impurity decrease* of an attribute  $A$  is then defined similarly to the gain in the entropy case

$$ImpDec(\mathcal{D}, A) = Gini(\mathcal{D}) - \sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Gini(\mathcal{D}_v)$$

In every step of the ID3 algorithm, we choose an attribute *maximizing* the impurity decrease for the current dataset  $\mathcal{D}$ .

# Gini Impurity

What is the intuition behind  $Gini(\mathcal{D})$  ?

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Assume we randomly independently choose objects from  $\mathcal{D}$ .

$1 - \sum_{c \in C} p_c^2$  is the probability of choosing two objects of different classes in two consecutive independent trials.

Indeed,  $p_c$  is the probability of choosing an object of class  $c$ ,  $p_c^2$  the probability of choosing objects of the class  $c$  twice, and  $\sum_{c \in C} p_c^2$  the probability of choosing two objects of the same class.

In what follows (and at the exam), we will work only with the Gini impurity as it is easier to compute by hand.

## Example

Consider our tennis example (see the table).

- ▶ Consider the whole dataset  $\mathcal{D}$ .
  - ▶  $p_{Yes} = 9/14$
  - ▶  $p_{No} = 5/14$
  - ▶  $Gini(\mathcal{D}) = 1 - (9/14)^2 - (5/14)^2 = 0.459$



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- ▶ For  $A = Outlook$  we get
  - ▶  $Gini(\mathcal{D}_{Sunny}) = 1 - (2/5)^2 - (3/5)^2 = 0.48$
  - ▶  $Gini(\mathcal{D}_{Overcast}) = 1 - 1^2 - 0^2 = 0$
  - ▶  $Gini(\mathcal{D}_{Rain}) = 1 - (3/5)^2 - (2/5)^2 = 0.48$

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Thus

$$\begin{aligned} ImpDec(\mathcal{D}, Outlook) &= \\ &0.459 - (5/14) \cdot 0.48 - (4/14) \cdot 0 - (5/14) \cdot 0.48 \\ &= 0.117 \end{aligned}$$

- ▶  $ImpDec(\mathcal{D}, Temperature) = 0.018$
- ▶  $ImpDec(\mathcal{D}, Humidity) = 0.091$
- ▶  $ImpDec(\mathcal{D}, Wind) = 0.030$

So the largest information gain is given by the *Outlook*.

## Example

Going further on, consider  $\mathcal{D} = \mathcal{D}_{Sunny}$ . We get

- ▶  $ImpDec(\mathcal{D}, Temperature) = 0.279$
- ▶  $ImpDec(\mathcal{D}, Humidity) = 0.48$
- ▶  $ImpDec(\mathcal{D}, Wind) = 0.013$

The best choice attribute after *Sunny* in *Outlook* is *Humidity*.

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Now consider  $\mathcal{D} = \mathcal{D}_{Rain}$ .

- ▶  $ImpDec(\mathcal{D}, Temperature) = 0.013$
- ▶  $ImpDec(\mathcal{D}, Humidity) = 0.013$
- ▶  $ImpDec(\mathcal{D}, Wind) = 0.48$

The best choice attribute after *Rain* in *Outlook* is *Wind*.

# Attribute Importance Computation

How important are attributes for the trained tree  $\mathcal{T}$ ? Depends on

- ▶ how close they are to the root of  $\mathcal{T}$ ,
- ▶ how large information gain/decrease in impurity they give.

There are several formulae for computing the importance.

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Then define the importance as the average decrease in Gini impurity (i.e., average *ImpDec*) in the nodes of  $T[A]$ :

$$GiniImportance(A) = \sum_{\tau \in T[A]} \frac{|\mathcal{D}[\tau]|}{|\mathcal{D}|} ImpDec(\mathcal{D}[\tau], A)$$

## Continuous-Valued Attributes

What if values of an attribute  $A$  come from a continuous variable?

$A$  is a numerical attribute that can take any value in an interval, such as temperature, size, time, etc.

## Continuous-Valued Attributes

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Consider an internal node  $\tau \in T_{int}$  assigned such a continuous attribute  $A$ . Then

- ▶  $\tau$  is assigned a threshold value called a *cut point*  $H \in \mathbb{R}$ ,
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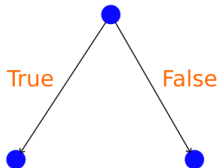
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During inference, when considering an example  $\vec{x}$  in the node  $\tau$ ,

- ▶ evaluate  $A(\vec{x}) \leq H$ ,
- ▶ if  $A(\vec{x}) \leq H$ , then follow  $e_{\text{true}}$ ,
- ▶ else follow  $e_{\text{false}}$ .

Temperature  $\leq 15$



In training, the cut point is chosen from the attribute values in the training set using information gain/impurity decrease similar to discrete attributes.

# Iris Example

**iris setosa**



petal

sepal

**iris versicolor**



petal

sepal

**iris virginica**



petal

sepal

## Attributes

Sepal.Length, Sepal.Width, Petal.Length, Petal.Width

## Classes (Variety)

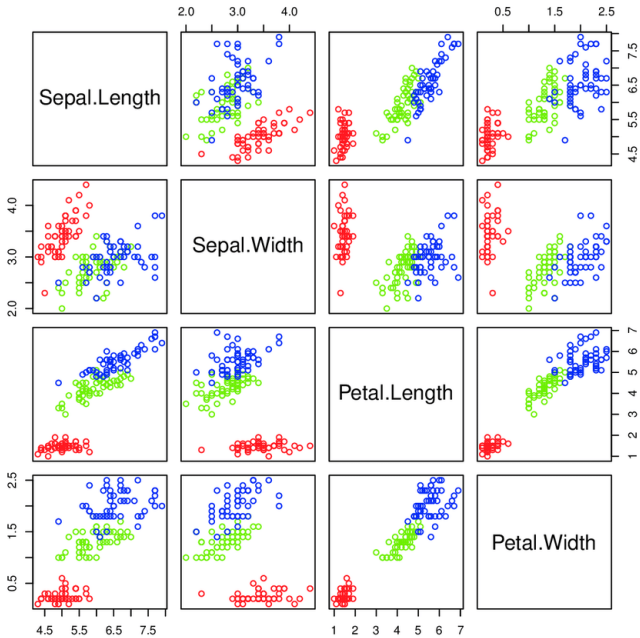
Setosa, Versicolor, Virginica

## Iris Example

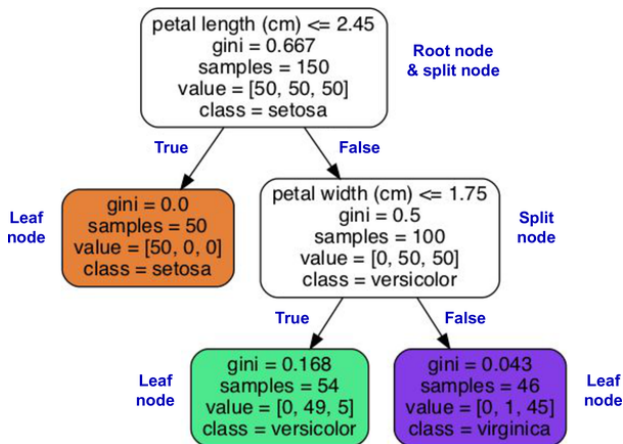
The dataset (150 examples):

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Variety
5.5	3.5	1.3	0.2	Setosa
6.8	2.8	4.8	1.4	Versicolor
6.7	3.1	4.7	1.5	Versicolor
6.9	3.1	5.1	2.3	Virginica
7.3	2.9	6.3	1.8	Virginica
5.4	3.7	1.5	0.2	Setosa
4.6	3.4	1.4	0.3	Setosa
6.2	2.8	4.8	1.8	Virginica
5.4	3.0	4.5	1.5	Versicolor
4.7	3.2	1.6	0.2	Setosa
6.7	3.3	5.7	2.1	Virginica
5.0	3.4	1.5	0.2	Setosa
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...				

# Iris Example

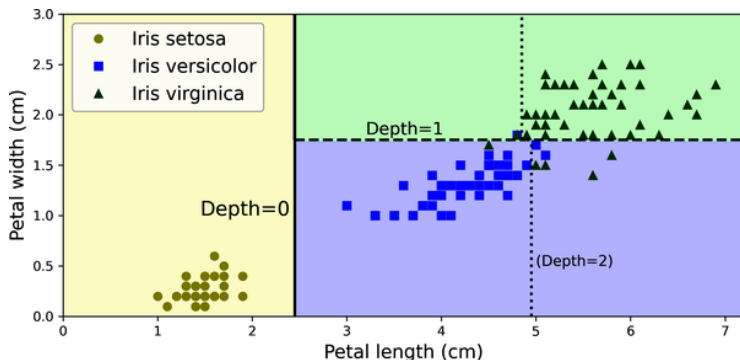


# Iris Example - Decision Tree



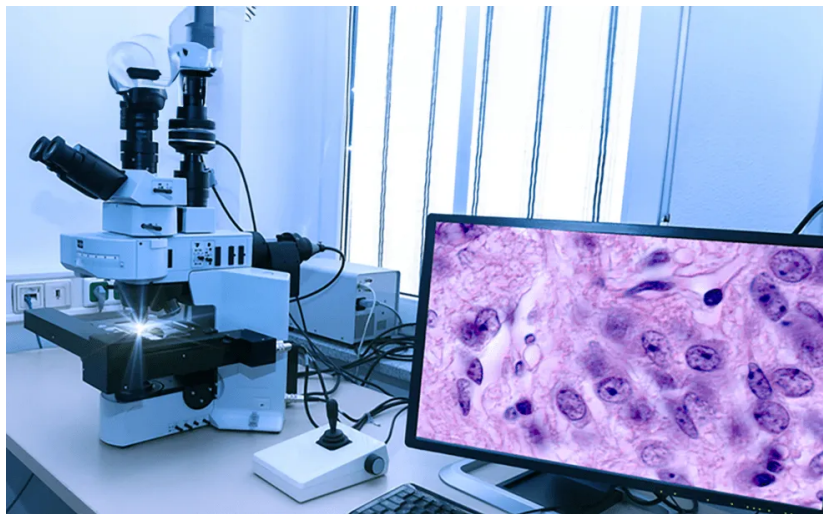


## Iris Example - Decision Tree Boudaries

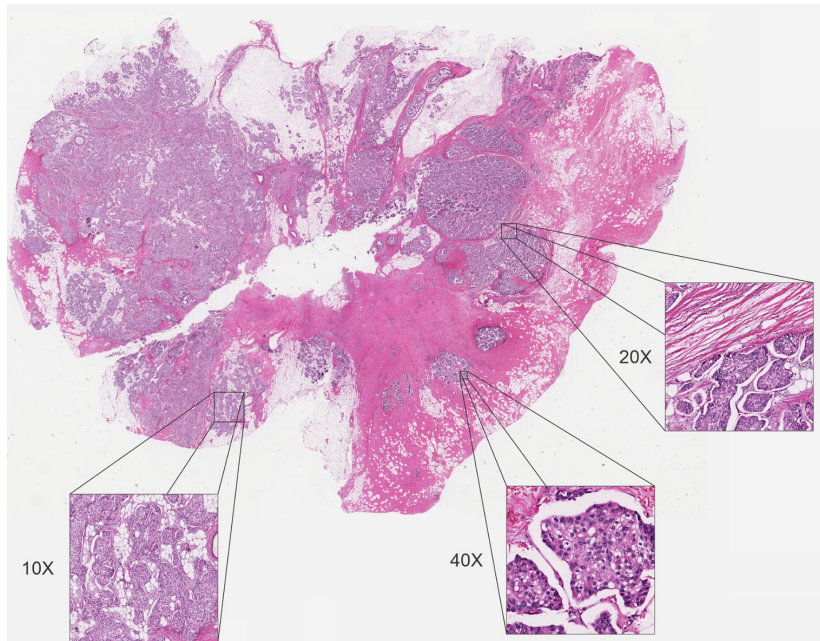


If the leaves are split further, the Depth = 2 boundary would be added.

## Example: Wisconsin Breast Cancer Dataset



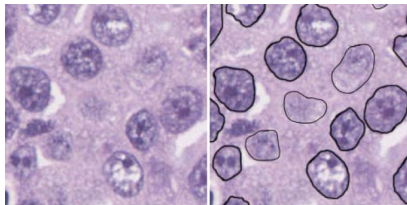
# Wisconsin Breast Cancer Dataset



## Example: Wisconsin Breast Cancer Dataset

- ▶ The Wisconsin Breast Cancer Dataset (WBCD) is used for binary classification of tumors.
- ▶ Origin: Created by Dr. William H. Wolberg at the University of Wisconsin-Madison.
- ▶ **Samples:** 569 breast cancer cases.
- ▶ **Target Variable:**
  - ▶ 0 = Benign (non-cancerous)
  - ▶ 1 = Malignant (cancerous)
- ▶ **Features:** 30 numerical attributes describing cell nuclei.

## Example: Wisconsin Breast Cancer Dataset



- ▶ Each sample is characterized by 10 different measurements:
  - ▶ Radius, Texture, Perimeter, Area
  - ▶ Smoothness, Compactness, Concavity
  - ▶ Concave Points, Symmetry, Fractal Dimension
- ▶ Each feature has three statistical measures:
  - ▶ Mean (Average over cells in the sample)
  - ▶ Standard Error (SE) (Variation within the sample)
  - ▶ Worst (Largest value in the sample)

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean	concave points_mean	...
0	842302	M	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	...
1	842517	M	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	...
2	84300903	M	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	...
3	84348301	M	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	...
4	84358402	M	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	...

## Example: Wisconsin Breast Cancer Dataset

Just asked ChatGPT: Train a decision tree predicting the diagnosis and show me graphically the result.

## Example: Wisconsin Breast Cancer Dataset

Just asked ChatGPT: Train a decision tree predicting the diagnosis and show me graphically the result.

I'll train a decision tree classifier to predict the **diagnosis** from your **cleaned\_breast\_cancer\_dataset.csv** and visualize the tree. Let me first inspect the dataset to confirm its structure.

The dataset has **569 samples** and **32 columns**, including an **ID column** and a **diagnosis column (target variable)**. The diagnosis is encoded as **1 (Malignant)** and **0 (Benign)**.

I will:

1. Remove the **ID** column.
2. Train a **Decision Tree Classifier** on the remaining features.
3. Visualize the trained tree.

(see the result shown separately; too large for a slide)

Training Accuracy: 0.9956

Test Accuracy: 0.9474

```

import pandas as pd
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.tree import DecisionTreeClassifier, plot_tree
from sklearn.metrics import accuracy_score

# Load dataset
file_path = "cleaned_breast_cancer_dataset.csv"
df = pd.read_csv(file_path)

# Remove ID column
df = df.drop(columns=["id"])

# Split data into features and target
X = df.drop(columns=["diagnosis"])
y = df["diagnosis"]

# Split into training and test sets
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42)

# Train decision tree classifier
clf = DecisionTreeClassifier(max_depth=4, random_state=42)
clf.fit(X_train, y_train)

# Evaluate model
train_accuracy = accuracy_score(y_train, clf.predict(X_train))
test_accuracy = accuracy_score(y_test, clf.predict(X_test))

# Print accuracy
print(f"Training Accuracy: {train_accuracy:.4f}")
print(f"Test Accuracy: {test_accuracy:.4f}")

# Plot decision tree
plt.figure(figsize=(20,10))
plot_tree(clf, feature_names=X.columns, class_names=["Benign", "Malignant"],
          filled=True, rounded=True)
plt.show()

```



# Decision Trees

## Practical Issues

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- ▶ Data preprocessing
- ▶ Model tuning (overfitting and underfitting)
- ▶ Sensitivity to changes in data/hyperparameters
- ▶ Learning representation problems (the XOR)

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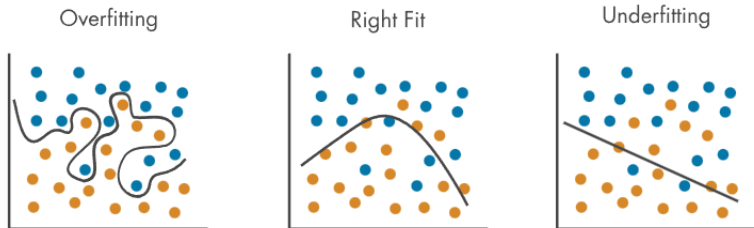
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Imbalanced classes might cause problems because of small information gain/impurity decrease in splitting.

# Model Tuning - Over/Under Fitting

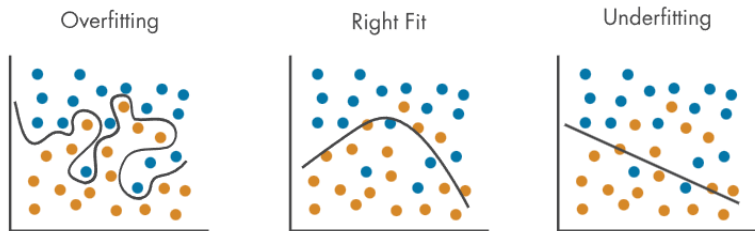
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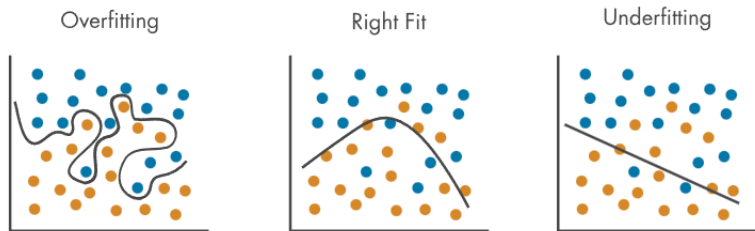
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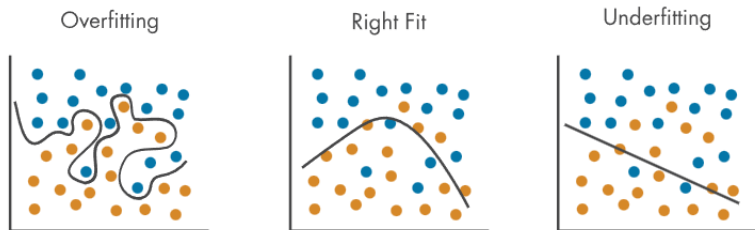
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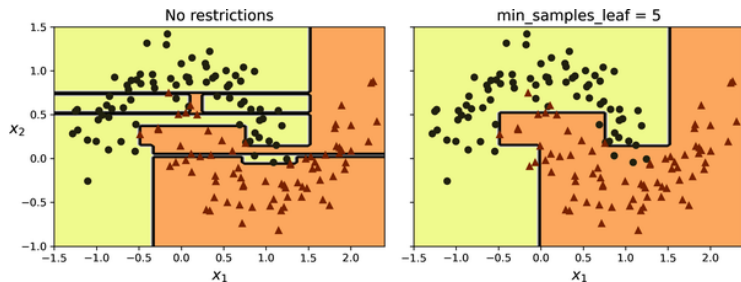
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- ▶ The middle one seems good (but still needs to be tested on fresh data).

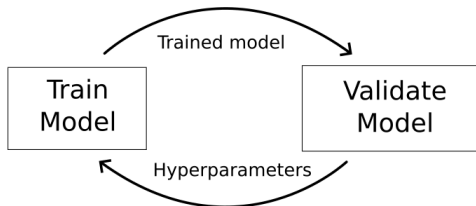
# Model Tuning - Overfitting in Decision Trees



See the overfitting on the left and the “nice” model on the right. Both overfitting and underfitting are best avoided. But how do we find out?

# Model Tuning (In General)

Recall from the first lecture:

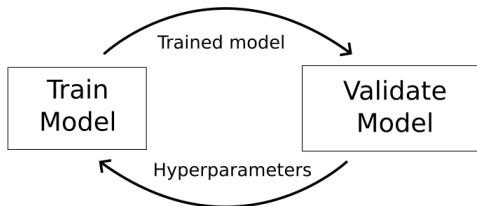


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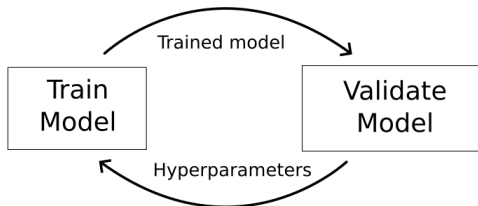
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What to observe? In the case of decision trees, one should observe the difference between performance measures (e.g., classification accuracy) on the training and validation sets.

The too-large difference implies an improperly fitting model.

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There are several approaches available for decision trees.

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The post-pruning approach has been more successful in practice than the pre-pruning because it is usually hard to say when to stop growing the tree.

We shall meet this controversy also in deep learning, where recent history shows a similar phenomenon.

The ensemble methods will be covered later when we discuss random forests.

# Pre-Pruning - Hyperparameters

Hyperparameters controlling the size of the tree:

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The deeper the tree, the more complex models you can create  $\Rightarrow$  overfitting. Low depth may restrict expressivity.

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- ▶ Minimum number of examples required to be in a leaf  
Similar to the previous one. A higher number means we cannot have very specific branches concerned with particular combinations of values.
- ▶ Minimum information gain/impurity decrease  
A small impurity decrease means that the split does not contribute too much to the classification (their proportions after a split are similar to proportions before a split). However, keep in mind that it is *weighted average impurity* after the split.



## Post-Pruning - Reduced Error Pruning

Train a large tree and then remove nodes that make classification worse on the validation set.

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Given a decision tree  $\mathcal{T}$  and its internal node  $\tau \in T_{int}$ , we denote by  $\mathcal{T}_{-\tau}$  the tree obtained from  $\mathcal{T}$  by removing the subtree rooted in  $\tau$ , i.e.,  $\tau$  is a leaf of  $\mathcal{T}_{-\tau}$ .

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```
1: Train  $\mathcal{T}$  to maximum fit on the training dataset.
2: while true do
3:    $Err[\mathcal{T}] \leftarrow$  the error of  $\mathcal{T}$  on the validation set.
4:   for  $\tau \in T_{int}$  do
5:      $Err[\mathcal{T}_{-\tau}] \leftarrow$  the error of  $\mathcal{T}_{-\tau}$  on the validation set.
6:   end for
7:   if  $Err[\mathcal{T}] \leq \min\{Err[\mathcal{T}_{-\tau}] \mid \tau \in T_{int}\}$  then return  $\mathcal{T}$ 
8:   else
9:      $\mathcal{T} \leftarrow \operatorname{argmin}\{Err[\mathcal{T}_{-\tau}] \mid \tau \in T_{int}\}$ 
10:  end if
11: end while
```

The error  $Err[\mathcal{T}]$  can be any measure of the “badness” of the decision tree  $\mathcal{T}$ . For example,  $1 - \text{Accuracy}$ .

## Other Pruning Methods

There are more pruning methods.

- ▶ Rule Post-Pruning:
  - ▶ Transform the tree into a set of rules.  
Rules correspond to paths in the tree; they have a form of implication: Specific values of attributes imply a class.
  - ▶ Remove the attribute conditions from the premises of the implications.

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Typically introduce regularization into the error functions:  
Given a decision tree  $\mathcal{T}$

$$Err_{\alpha}(\mathcal{T}) = Err(\mathcal{T}) + \alpha|\mathcal{T}|$$

The original paper by Breiman et al. (1984) defined  $Err(\mathcal{T})$  to be the misclassification rate on the training dataset, and  $|\mathcal{T}|$  is the number of nodes of the tree  $\mathcal{T}$ .

# Sensitivity to Small Changes and Randomness

- ▶ Decision trees are sensitive to small changes in data and hyperparameters.  
Several attributes may provide (almost) identical information gain but divide the training dataset very differently.
- ▶ Some implementations choose attributes partially in random (sci-kit-learn). You may get completely different trees.

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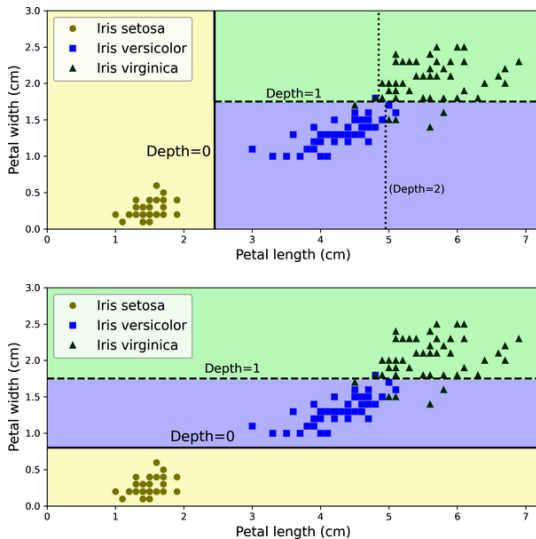
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A solution is to train an ensemble of many decision trees and then use majority voting for classification.

This is the fundamental idea behind random forests (see later lectures).



# Iris - Illustration

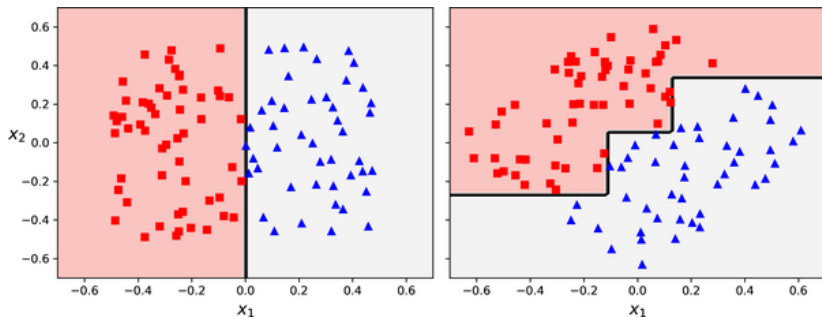


Decision trees trained on the Iris dataset.

Iris Setosa is perfectly separated by many choices for the first split.

# Axis Sensitivity

The decision makes divisions along particular axes:

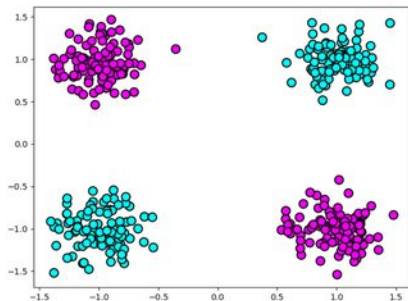


That is, rotated data may result in a completely different model.

That is why decision trees are often preceded by the *principal component analysis (PCA)* transformation, which aligns data along the axes of maximum data variance.

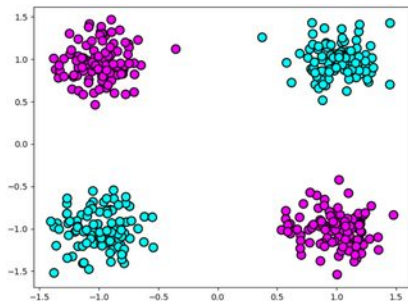
# XOR Training Problem

Consider the following training dataset:

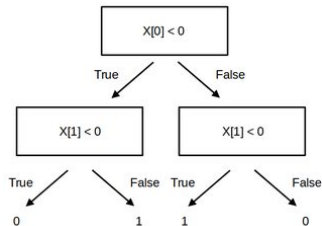


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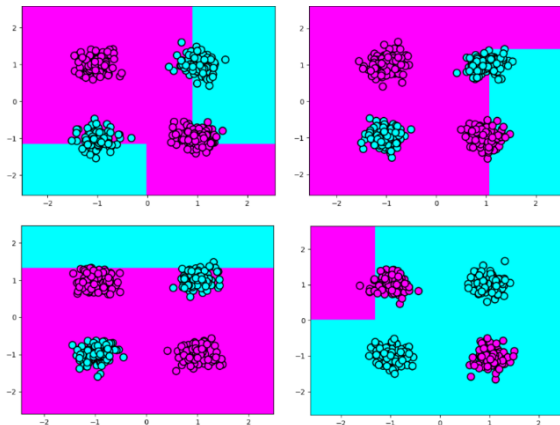


An ideal decision tree would look like this:



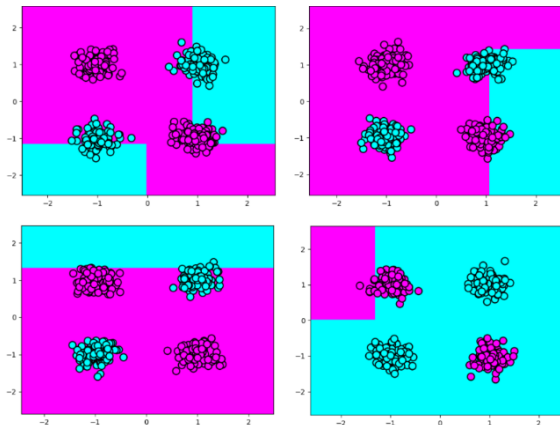
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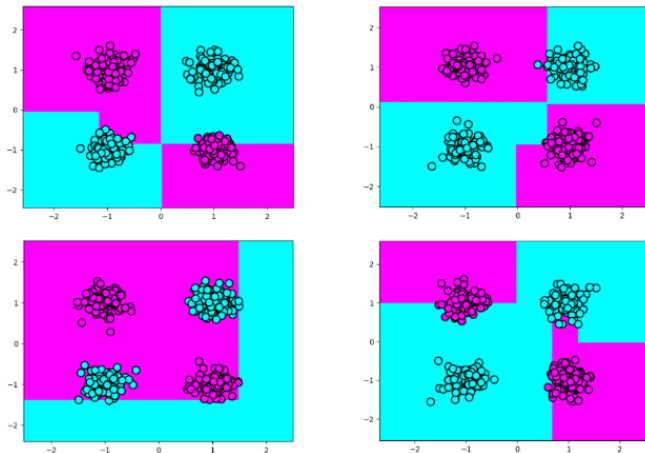


The problem: Both information gain and decrease in impurity consider only the relationship of a *single* attribute and the class.

However, there is no relationship between a single attribute and the class; both attributes need to be considered together!

# More Attempts at Training on XOR

Max depth = 3:



It's better but still fails occasionally.

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- ▶ The cost of using a well-balanced tree is logarithmic in the number of data points used to train it.

## Disadvantages of Decision Trees

- ▶ Overfitting: Trees can be over-complex and not generalize well, needing pruning or limits on tree depth.
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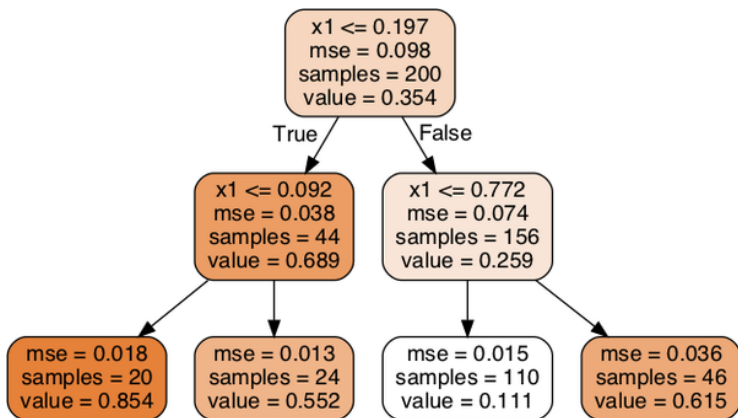
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- ▶ Difficulty learning certain concepts, such as XOR.
- ▶ Bias in trees: Decision trees can create biased trees if some classes dominate. Balancing the dataset is recommended.
- ▶ Learning optimal trees is NP-complete: Heuristic algorithms like greedy algorithms are used, which do not guarantee globally optimal trees. Ensemble methods can help.

# History of Decision Trees

- ▶ Hunt and colleagues use exhaustive search decision-tree methods (CLS) to model human concept learning in the 1960's.
- ▶ In the late 70's, Quinlan developed ID3 with the information gain heuristic to learn expert systems from examples.
- ▶ Simultaneously, Breiman, Friedman, and colleagues develop CART (Classification and Regression Trees), similar to ID3.
- ▶ In the 1980s, various improvements were introduced to handle noise, continuous features, missing features, and improved splitting criteria. Various expert-system development tools results.
- ▶ Quinlan's updated decision-tree package (C4.5) released in 1993.

## Comment on Regression Trees

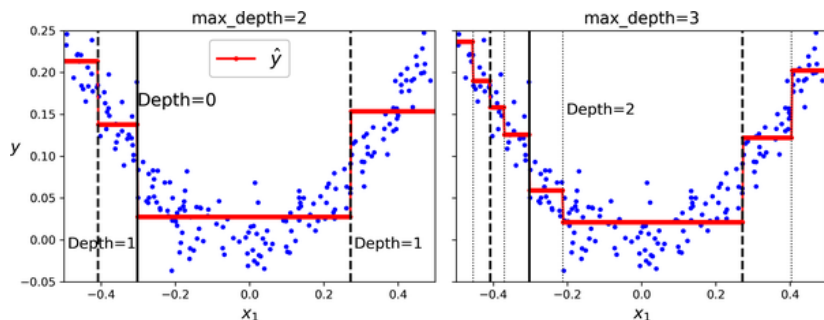
Decision trees can also be used to approximate functions. Assign a function value to the leaves instead of classes.



Here, “mse” is the mean-squared-error.



# Comment on Regression Trees



Intuitively, for every subinterval of  $x_1$ , the value (the red line) is at the average  $y$  over the subinterval.

How are the subintervals being set?

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A *regression tree* is a decision tree whose leaves are labeled by values from  $\mathbb{R}$ .

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The training procedure is the same as for the decision trees, except that the splits and cut points are selected differently.

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Given a dataset  $\mathcal{D} = \{(\vec{x}_1, d_1), \dots, (\vec{x}_p, d_p)\}$ , we denote by  $\bar{\mathcal{D}}$  the average *desired* value in  $\mathcal{D}$ , that is  $\bar{\mathcal{D}} = \frac{1}{p} \sum_{k=1}^p d_k$ .

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$$\mathcal{D}_{\leq H} = \{(\vec{x}, d) \in \mathcal{D} \mid A(\vec{x}) \leq H\} \quad \mathcal{D}_{> H} = \{(\vec{x}, d) \in \mathcal{D} \mid A(\vec{x}) > H\}$$

Minimizes the following *split error*:

$$\frac{1}{|\mathcal{D}|} \left( \sum_{(\vec{x}, d) \in \mathcal{D}_{\leq H}} (d - \bar{D}_{\leq H})^2 + \sum_{(\vec{x}, d) \in \mathcal{D}_{> H}} (d - \bar{D}_{> H})^2 \right)$$

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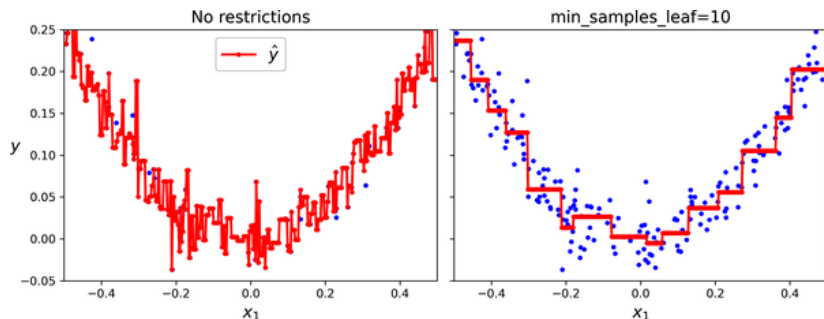
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If  $\Delta$  is large enough, split on  $A$  and  $H$  that minimize the split error. Otherwise, stop splitting and label the leaf with  $\bar{D}$ .

# Regression Tress

Without any lower bound on the number of examples in the leaves, the algorithm will eventually overfit by splitting into (possibly) singleton leaves.



# Probabilistic Classification

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The degree of belief (Bayesian), or the relative frequency (frequentists), is the *probability*.

# Basic Discrete Probability Theory

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- ▶ **Basic laws:**  $P(\Omega) = 1$ ,  $P(\emptyset) = 0$ , given disjoint sets  $A, B$  we have  $P(A \cup B) = P(A) + P(B)$ ,  $P(\Omega \setminus A) = 1 - P(A)$ .

# Conditional Probability and Independence

- ▶  $P(A \mid B)$  is the probability of  $A$  given  $B$  (assume  $P(B) > 0$ ) defined by

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- ▶  $A$  and  $B$  are **independent** if  $P(A \cap B) = P(A) \cdot P(B)$ .

It is easy to show that if  $P(B) > 0$ , then

$A, B$  are independent iff  $P(A \mid B) = P(A)$ .

# Random Variables and Random Vectors

- ▶ A *random variable*  $X$  is a function  $X : \Omega \rightarrow \mathbb{R}$ .  
A dice:  $X : \{1, \dots, 6\} \rightarrow \{0, 1\}$  such that  $X(n) = n \bmod 2$ .
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We use  $X = (X_1, \dots, X_d)$  where  $X_i$  is a random variable returning the  $i$ -th component of  $X$ .

- ▶ Consider random variables  $X_1, X_2$  and  $Y$ . The variables  $X_1, X_2$  are *conditionally independent given  $Y$*  if for all  $x_1, x_2$  and  $y$  we have that

$$P(X_1 = x_1, X_2 = x_2 \mid Y = y) = \\ P(X_1 = x_1 \mid Y = y) \cdot P(X_2 = x_2 \mid Y = y)$$

## Random Vectors – Example

Let  $\Omega$  be a space of colored geometric shapes that are divided into two categories (**1** and **0**).

Assume a random vector  $X = (X_{color}, X_{shape}, X_{cat})$  where

- ▶  $X_{color} : \Omega \rightarrow \{red, blue\}$ ,
- ▶  $X_{shape} : \Omega \rightarrow \{circle, square\}$ ,
- ▶  $X_{cat} : \Omega \rightarrow \{\mathbf{1}, \mathbf{0}\}$ .

The following tables give probability distribution of values:

category **1**:

	circle	square
red	0.2	0.02
blue	0.02	0.01

category **0**:

	circle	square
red	0.05	0.3
blue	0.2	0.2

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Example:

$$P(\text{red}, \text{circle}, \mathbf{1}) = P(X_{\text{color}} = \text{red}, X_{\text{shape}} = \text{circle}, X_{\text{cat}} = \mathbf{1}) = 0.2$$

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"Summing over" all possible values of some variable(s) gives the distribution of the rest:

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$$P(\text{red}) = 0.2 + 0.02 + 0.05 + 0.3 = 0.57$$

Thus also, all conditional probabilities can be computed:

$$P(\mathbf{1} \mid \text{red}, \text{circle}) = \frac{P(\text{red}, \text{circle}, \mathbf{1})}{P(\text{red}, \text{circle})} = \frac{0.2}{0.25} = 0.8$$



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**Bayes classifier:** Given a vector of feature values  $\vec{x}$ ,

$$C^{Bayes}(\vec{x}) := \begin{cases} \mathbf{1} & \text{if } P(Y = \mathbf{1} \mid X = \vec{x}) \geq P(Y = \mathbf{0} \mid X = \vec{x}) \\ \mathbf{0} & \text{otherwise.} \end{cases}$$

Intuitively,  $C^{Bayes}$  assigns to  $\vec{x}$  the most probable category it might be in.

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The Bayes classifier compares  $P(Y = 1 \mid X = (40g, 5cm))$  with  $P(Y = 0 \mid X = (40g, 5cm))$  and selects the more probable category given the features.

**Crucial question:** Is such a classifier good?

There are other classifiers, e.g., one which compares the weight divided by 10 with the diameter and decides based on the answer, or maybe a classifier that sums the weight and the diameter and compares the result with a constant, etc.



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Define the error of the classifier  $C$  by

$$E_C = P(Y \neq C)$$

(Here we slightly abuse notation and apply  $C$  to samples, technically we apply the composition  $C \circ X$  of  $C$  and  $X$  which first determines the features using  $X$  and then classifies according to  $C$ ).

# Bayes Classifier

Let  $C$  be an arbitrary *classifier*, that is a function that to every feature vector  $\vec{x} \in \mathbb{R}^n$  assigns a class from  $\{\mathbf{0}, \mathbf{1}\}$ .

Define the error of the classifier  $C$  by

$$E_C = P(Y \neq C)$$

(Here we slightly abuse notation and apply  $C$  to samples, technically we apply the composition  $C \circ X$  of  $C$  and  $X$  which first determines the features using  $X$  and then classifies according to  $C$ ).

## Theorem

The Bayes classifier  $C^{Bayes}$  minimizes  $E_C$ , that is

$$E_{C^{Bayes}} = \min_{C \text{ is a classifier}} E_C$$

## Practical Use of Bayes Classifier

**The crucial problem:** The probability  $P$  is not known!

In particular, where to get  $P(Y = \mathbf{1} \mid X = \vec{x})$  ?

Note that  $P(Y = \mathbf{0} \mid X = \vec{x}) = 1 - P(Y = \mathbf{1} \mid X = \vec{x})$

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Where do you get these probabilities?

In some cases, the probabilities might come from the knowledge of the solved problem (e.g., applications in physics might be supported by a theory giving the probabilities).

In most cases, however,  $P$  is estimated from sampled data by

$$\bar{P}(Y = \mathbf{1} \mid X = \vec{x}) = \frac{\text{number of samples with } Y = \mathbf{1} \text{ and } X = \vec{x}}{\text{number of samples with } X = \vec{x}}$$

(We use  $\bar{P}$  to denote an estimate of  $P$  from data.)

## Estimating $P$

Consider a problem with  $X = (X_1, X_2, X_3)$  where each  $X_i$  returns either 0 or 1. What might the data look like?

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Part of the data table:

$Y$	$X_1$	$X_2$	$X_3$
<b>1</b>	1	0	1
<b>1</b>	0	1	1
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<b>0</b>	1	1	1
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All data with  $X_1 = 1, X_2 = 0, X_3 = 1$ :

$Y$	$X_1$	$X_2$	$X_3$
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The probability table and the necessary data are typically too large!

Concretely, if all  $X_1, \dots, X_n$  are binary, there are  $2^n$  probabilities  $P(Y = \mathbf{1} \mid X = \vec{x})$ , one for each possible  $\vec{x} \in \{0, 1\}^n$ .

# Let's Look at It the Other Way Round

Theorem (Bayes,1764)

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Proof.

$$P(A | B) = \frac{P(A \cap B)}{P(B)} = \frac{\frac{P(A \cap B)}{P(A)} \cdot P(A)}{P(B)} = \frac{P(B | A) \cdot P(A)}{P(B)}$$



# Bayesian Classification

Determine the category for  $\vec{x}$  by computing

$$P(Y = y \mid X = \vec{x}) = \frac{P(Y = y) \cdot P(X = \vec{x} \mid Y = y)}{P(X = \vec{x})}$$

for both  $y \in \{\mathbf{0}, \mathbf{1}\}$  and deciding whether or not the following holds:

$$P(Y = \mathbf{1} \mid X = \vec{x}) \geq P(Y = \mathbf{0} \mid X = \vec{x})$$

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So, to make the classifier, we need to compute the following:

- ▶ **The prior**  $P(Y = \mathbf{1})$  (then  $P(Y = \mathbf{0}) = 1 - P(Y = \mathbf{1})$ )
- ▶ **The conditionals**  $P(X = \vec{x} \mid Y = y)$  for  $y \in \{\mathbf{0}, \mathbf{1}\}$  and for every  $\vec{x}$

## Estimating the Prior and Conditionals

- ▶  $P(Y = \mathbf{1})$  can be easily estimated from data by

$$\bar{P}(Y = \mathbf{1}) = \frac{\text{number of samples with } Y = \mathbf{1}}{\text{number of all samples}}$$

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- ▶ If the dimension of features is small,  $P(X = \vec{x} \mid Y = y)$  can be estimated from data similarly as  $P(Y = \mathbf{1} \mid X = \vec{x})$  by

$$\bar{P}(X = \vec{x} \mid Y = y) = \frac{\text{number of samples with } Y = y \text{ and } X = \vec{x}}{\text{number of samples with } Y = y}$$

Unfortunately, for higher dimensional data too many samples are needed to estimate all  $P(X = \vec{x} \mid Y = y)$  (there are too many  $\vec{x}$ 's).

So where is the advantage of using the Bayes thm.??

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We introduce *independence assumptions* about the features!



# Naive Bayes

- ▶ We assume that features are (conditionally) independent *given the category*. That is for all  $\vec{x} = (x_1, \dots, x_n)$  and  $y \in \{0, 1\}$  we **assume**:

$$\begin{aligned} P(X = x \mid Y = y) &= P(X_1 = x_1, \dots, X_n = x_n \mid Y) \\ &= \prod_{i=1}^n P(X_i = x_i \mid Y = y) \end{aligned}$$

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- ▶ Therefore, we only need to specify  $P(X_i = x_i \mid Y = y)$  for each possible pair of a feature-value  $x_i$  and  $y \in \{0, 1\}$ .

Note that if all  $X_i$  are binary (values in  $\{0, 1\}$ ), this requires specifying only  $2n$  parameters:

$$P(X_i = 1 \mid Y = \mathbf{1}) \text{ and } P(X_i = 1 \mid Y = \mathbf{0}) \text{ for each } X_i$$

as  $P(X_i = 0 \mid Y = y) = 1 - P(X_i = 1 \mid Y = y)$  for  $y \in \{0, 1\}$ .

Compared to specifying  $2^n$  parameters without any independence assumption.

## Estimating the marginal probabilities

Estimate the probabilities  $P(X_i = x_i \mid Y = y)$  by

$$\bar{P}(X_i = x_i \mid Y = y) = \frac{\text{number of samples with } X_i = x_i \text{ and } Y = y}{\text{number of samples with } Y = y}$$

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Estimate the probabilities  $P(X_i = x_i \mid Y = y)$  by

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**Example:** Consider a problem with  $X = (X_1, X_2, X_3)$  where each  $X_i$  returns either 0 or 1. The data is

$Y$	$X_1$	$X_2$	$X_3$
<b>1</b>	1	0	1
<b>1</b>	0	1	1
<b>0</b>	1	0	1
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$$\bar{P}(X_1 = 1 \mid Y = \mathbf{1}) = 1/3 \quad \bar{P}(X_1 = 1 \mid Y = \mathbf{0}) = 2/3$$

$$\bar{P}(X_2 = 1 \mid Y = \mathbf{1}) = 1/3 \quad \bar{P}(X_2 = 1 \mid Y = \mathbf{0}) = 1/3$$

$$\bar{P}(X_3 = 1 \mid Y = \mathbf{1}) = 2/3 \quad \bar{P}(X_3 = 1 \mid Y = \mathbf{0}) = 1$$

## Naive Bayes – Example

Consider classification of geometric shapes:

$X_1 \in \{small, medium, large\}$

$X_2 \in \{red, blue, green\}$

$X_3 \in \{square, triangle, circle\}$

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Consider classification of geometric shapes:

$X_1 \in \{small, medium, large\}$

$X_2 \in \{red, blue, green\}$

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Assume that we have already estimated the following probabilities:

	$Y = \mathbf{1}$	$Y = \mathbf{0}$
$\bar{P}(Y)$	0.5	0.5
$\bar{P}(small \mid Y)$	0.4	0.4
$\bar{P}(medium \mid Y)$	0.1	0.2
$\bar{P}(large \mid Y)$	0.5	0.4
$\bar{P}(red \mid Y)$	0.9	0.3
$\bar{P}(blue \mid Y)$	0.05	0.3
$\bar{P}(green \mid Y)$	0.05	0.4
$\bar{P}(square \mid Y)$	0.05	0.4
$\bar{P}(triangle \mid Y)$	0.05	0.3
$\bar{P}(circle \mid Y)$	0.9	0.3

Does  $(medium, red, circle)$  belong to the category **1** ?

	$Y = \mathbf{1}$	$Y = \mathbf{0}$
$\bar{P}(Y)$	0.5	0.5
$\bar{P}(\textit{medium} \mid Y)$	0.1	0.2
$\bar{P}(\textit{red} \mid Y)$	0.9	0.3
$\bar{P}(\textit{circle} \mid Y)$	0.9	0.3

Denote  $\vec{x} = (\textit{medium}, \textit{red}, \textit{circle})$ .



	$Y = \mathbf{1}$	$Y = \mathbf{0}$
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Denote  $\vec{x} = (\textit{medium}, \textit{red}, \textit{circle})$ .

$$\begin{aligned}
 P(Y = \mathbf{1} \mid X = \vec{x}) &= \\
 &= P(\mathbf{1}) \cdot P(\textit{medium} \mid \mathbf{1}) \cdot P(\textit{red} \mid \mathbf{1}) \cdot P(\textit{circle} \mid \mathbf{1}) / P(X = \vec{x}) \\
 &\doteq 0.5 \cdot 0.1 \cdot 0.9 \cdot 0.9 / P(X = \vec{x}) = 0.0405 / P(X = \vec{x})
 \end{aligned}$$

	$Y = \mathbf{1}$	$Y = \mathbf{0}$
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 &= P(\mathbf{0}) \cdot P(\text{medium} \mid \mathbf{0}) \cdot P(\text{red} \mid \mathbf{0}) \cdot P(\text{circle} \mid \mathbf{0}) / P(X = \vec{x}) \\
 &\doteq 0.5 \cdot 0.2 \cdot 0.3 \cdot 0.3 / P(X = \vec{x}) = 0.009 / P(X = \vec{x})
 \end{aligned}$$

(Note that we used the estimates  $\bar{P}$  of  $P$  to finish the computation above.)

	$Y = \mathbf{1}$	$Y = \mathbf{0}$
$\bar{P}(Y)$	0.5	0.5
$\bar{P}(\text{medium} \mid Y)$	0.1	0.2
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Denote  $\vec{x} = (\text{medium}, \text{red}, \text{circle})$ .

$$\begin{aligned}
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Apparently,

$$P(Y = \mathbf{1} \mid X = \vec{x}) \doteq 0.0405 / P(X = \vec{x}) > 0.009 / P(X = \vec{x}) \doteq P(\mathbf{0} \mid X = \vec{x})$$

So we classify  $\vec{x}$  to the category  $\mathbf{1}$ .

## Estimating Probabilities in Practice

We already know that  $P(X_i = x_i \mid Y = y)$  can be estimated by

$$\bar{P}(X_i = x_i \mid Y = y) = \ell_{y,x_i} / \ell_y$$

where

- ▶  $\ell_{y,x_i}$  = number of samples with  $Y = y$  and  $X_i = x_i$
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**Problem:** If, by chance, a rare value  $x_i$  of a feature  $X_i$  never occurs in the training data, we get

$$\bar{P}(X_i = x_i \mid Y = y) = 0 \quad \text{for both } y \in \{\mathbf{0}, \mathbf{1}\}$$

But then  $\bar{P}(X = x) = 0$  for  $x$  containing the value  $x_i$  for  $X_i$ , and thus  $\bar{P}(Y = y \mid X = x)$  is not well defined.

Moreover,  $\bar{P}(Y = y) \cdot \bar{P}(X = x \mid Y = y) = 0$  (for  $y \in \{\mathbf{0}, \mathbf{1}\}$ ) so even this cannot be used for classification.

# Probability Estimation Example

Training data:

Size	Color	Shape	Class
small	red	circle	<b>1</b>
large	red	circle	<b>1</b>
small	red	triangle	<b>0</b>
large	blue	circle	<b>0</b>

Estimated probabilities:

	<b><math>Y = 1</math></b>	<b><math>Y = 0</math></b>
$\bar{P}(Y)$	0.5	0.5
$\bar{P}(\text{small} \mid Y)$	0.5	0.5
$\bar{P}(\text{medium} \mid Y)$	0	0
$\bar{P}(\text{large} \mid Y)$	0.5	0.5
$\bar{P}(\text{red} \mid Y)$	1	0.5
$\bar{P}(\text{blue} \mid Y)$	0	0.5
$\bar{P}(\text{green} \mid Y)$	0	0
$\bar{P}(\text{square} \mid Y)$	0	0
$\bar{P}(\text{triangle} \mid Y)$	0	0.5
$\bar{P}(\text{circle} \mid Y)$	1	0.5

Note that  $\bar{P}(\text{medium} \mid \mathbf{1}) = P(\text{medium} \mid \mathbf{0}) = 0$  and thus also  $\bar{P}(\text{medium}, \text{red}, \text{circle}) = 0$ .

So what is  $\bar{P}(\mathbf{1} \mid \text{medium}, \text{red}, \text{circle})$  ?

## Smoothing

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- ▶ To account for estimation from small samples, probability estimates are adjusted or *smoothed*.
- ▶ *Laplace smoothing* adds one to every count of feature values

$$\tilde{P}(X_i = x_i \mid Y = y) = \frac{\ell_{y,x_i} + 1}{\ell_y + v_i}$$

where

- ▶  $\ell_y$  = number of training samples with  $Y = y$ ,
- ▶  $\ell_{y,x_i}$  = number of training samples with  $Y = y$  and  $X_i = x_i$ ,
- ▶  $v_i$  is the number of all distinct values of the variable  $X_i$ .

To understand note that

$$\ell_y = \sum_{x_i \text{ is a value of } X_i} \ell_{y,x_i}$$

and thus

$$\bar{P}(X_i = x_i \mid Y = y) = \ell_{y,x_i} / \sum_{x_i \text{ is a value of } X_i} \ell_{y,x_i}$$

$$\tilde{P}(X_i = x_i \mid Y = y) = (\ell_{y,x_i} + 1) / \sum_{x_i \text{ is a value of } X_i} (\ell_{y,x_i} + 1)$$



# Laplace Smoothing Example

- ▶ Assume training set contains 10 samples of category **1**:
  - ▶ 4 small
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- ▶ Assume training set contains 10 samples of category **1**:
  - ▶ 4 small
  - ▶ 0 medium
  - ▶ 6 large
- ▶ Estimate parameters as follows
  - ▶  $\tilde{P}(\text{small} \mid \mathbf{1}) = (4 + 1)/(10 + 3) = 0.384$
  - ▶  $\tilde{P}(\text{medium} \mid \mathbf{1}) = (0 + 1)/(10 + 3) = 0.0769$
  - ▶  $\tilde{P}(\text{large} \mid \mathbf{1}) = (6 + 1)/(10 + 3) = 0.538$

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A random variable  $X : \Omega \rightarrow \mathbb{R}^+$  has a density  $p : \mathbb{R} \rightarrow \mathbb{R}^+$  if for every interval  $[a, b]$  we have

$$P(a \leq X \leq b) = \int_a^b p(x) dx$$

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Usually,  $P(X_i | Y = y)$  is used to denote the *density* of  $X_i$  conditioned on  $Y = y$ .

- ▶ The densities  $P(X_i | Y = y)$  are usually estimated using Gaussian densities as follows:
  - ▶ Estimate the mean  $\mu_{iy}$  and the standard deviation  $\sigma_{iy}$  based on training data.
  - ▶ Then put

$$\bar{P}(X_i | Y = y) = \frac{1}{\sigma_{iy} \sqrt{2\pi}} \exp \left( \frac{-(X_i - \mu_{iy})^2}{2\sigma_{iy}^2} \right)$$

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- ▶ Experiments show that it is quite competitive with other classification methods.  
Even if the probabilities are not accurately estimated, it often picks the correct maximum probability category.
- ▶ Directly constructs a model from parameter estimates that are calculated from the training data.
- ▶ Typically handles outliers and noise well in the discrete version. In the continuous case depends on the way the parameters are estimated (e.g., the mean is very sensitive to outliers).

# Comments on Naive Bayes

- ▶ Tends to work well despite rather a strong assumption of conditional independence of features.
- ▶ Experiments show that it is quite competitive with other classification methods.  
Even if the probabilities are not accurately estimated, it often picks the correct maximum probability category.
- ▶ Directly constructs a model from parameter estimates that are calculated from the training data.
- ▶ Typically handles outliers and noise well in the discrete version. In the continuous case depends on the way the parameters are estimated (e.g., the mean is very sensitive to outliers).
- ▶ Missing values are easy to deal with; use only non-missing values in the computation of  $\bar{P}(X_i = x_i \mid Y = y)$ .

## Bayesian Networks (Basic Information)

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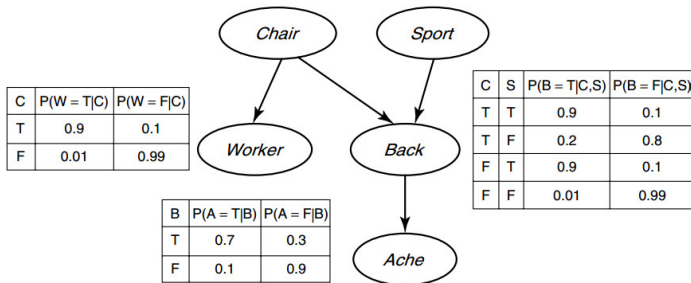
(But now in a well-defined sense.)

Bayesian networks are a graphical model that uses a directed acyclic graph to specify dependencies among variables.

## Bayesian Networks – Example

$P(C = T)$	$P(C = F)$
0.8	0.2

$P(S = T)$	$P(S = F)$
0.02	0.98



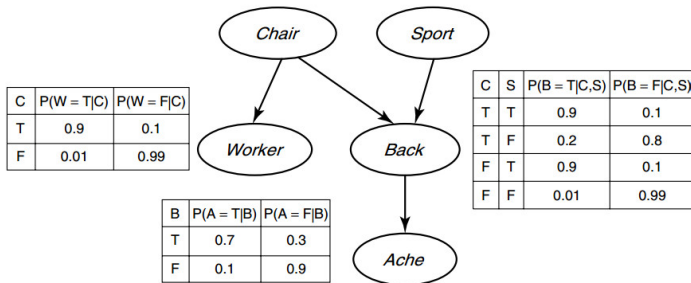
Now, e.g.,

$$P(C, S, W, B, A) = P(C) \cdot P(S) \cdot P(W | C) \cdot P(B | C, S) \cdot P(A | B)$$

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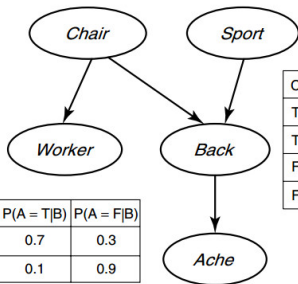
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C	$P(W = T C)$	$P(W = F C)$
T	0.9	0.1
F	0.01	0.99

B	$P(A = T B)$	$P(A = F B)$
T	0.7	0.3
F	0.1	0.9

C	S	$P(B = T C,S)$	$P(B = F C,S)$
T	T	0.9	0.1
T	F	0.2	0.8
F	T	0.9	0.1
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Now, we may, e.g., infer the probability  $P(C = T | A = T)$  that we sit in the wrong chair, assuming that our back aches.

We have to store only 10 numbers as opposed to  $2^5 - 1$  possible probabilities for all vectors of values of  $C, S, W, B, A$ .

# Bayesian Networks – Learning & Naive Bayes

Many algorithms have been developed for learning:

- ▶ the structure of the graph of the network,
- ▶ the *conditional probability tables*.

The methods are based on maximum-likelihood estimation, gradient descent, etc.

Automatic procedures are usually combined with expert knowledge.

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Can you express the naive Bayes for  $Y, X_1, \dots, X_n$  using a Bayesian network?

# Classifier Evaluation

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Assume binary classification into two classes  $\{0, 1\}$ .

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There are many possible metrics ...

I will call the class 1 *positive* and the class 0 *negative*.

Note that the class 0 is not negative in the numerical sense but in the absence of something (e.g., predicted illness).

# Confusion Matrix for Binary Classifier

		Predicted	
		1	0
Actual	1	TP	FN
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Index	1	2	3	4	5	6	7	8	9	10	11	12
Actual	1	1	1	1	1	1	1	1	0	0	0	0
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Result	FN	FN	TP	TP	TP	TP	TP	TP	FP	TN	TN	TN



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## Terminology

- ▶ TP aka hit
- ▶ TN aka correct rejection
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In what follows, we also use

- ▶  $P = TP + FN$  of all cases with the *actual* class 1
- ▶  $N = TN + FP$  of all cases with the *actual* class 0
- ▶  $PP = TP + FP$  of all cases with the *predicted* class 1
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There is a large number of derived metrics. We consider some of the most used in practice.

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The Accuracy is

$$\text{ACC} = \frac{TP + TN}{P + N} = \frac{6 + 3}{12} = \frac{3}{4}$$

## Accuracy - Imbalanced Classes

Accuracy can be misleading when the classes are imbalanced:

- ▶ Consider 100 cases, 90 in the class 0 and 10 in the class 1,
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However, the classifier is pretty bad in the positive cases.

In the case of cancer prediction, such a classifier would be a disaster.

# Precision & Recall

To mitigate the defect of the Accuracy, we may compute the following metrics:

$$\text{Precision} = \frac{TP}{PP} \quad (= \text{how often is predicted positive actually positive})$$

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$$\text{Recall} = \frac{TP}{P} \quad (= \text{how often is actually positive predicted positive})$$

Recall is also known as true positive rate, sensitivity, hit rate, and power.

## Precision & Recall - Example

**Example:** In our cancer example:

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- ▶ Precision measures how often is the patient predicted to be ill truly ill (in our case, 6/7)
- ▶ Recall measures how often is an ill patient found to be ill (in our case, 6/8)



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$$\text{Precision} = 1$$

$$\text{Recall} = \frac{1}{10}$$

You can see that the predictor is very precise (on the class 1) but useless due to the weak Recall.

## Precision & Recall - Relative Importance

Let us get back to our cancer example:

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By now, you should remember what they measure.

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Consider *Precision* and *Recall*.

By now, you should remember what they measure.

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Which of the two is more important for plagiarism detectors?

Can we get a single number summarizing both Precision and Recall?

For example, to compare two classifiers.

## $F_1$ Score

$F_1$  score is the harmonic mean of Recall and Precision:

$$F_1 = \frac{2}{\text{Recall}^{-1} + \text{Precision}^{-1}} = \frac{2TP}{2TP + FP + FN}$$

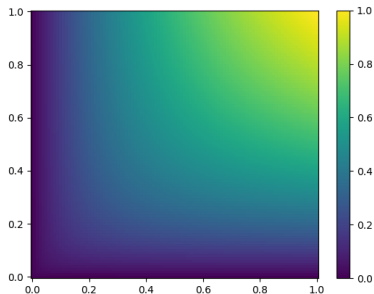
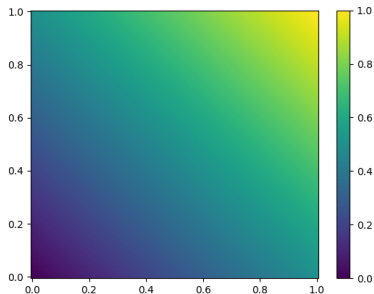


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Compare the arithmetic (left) and harmonic (right) mean:



The harmonic mean prefers the two values closer to each other.

For example, the harmonic mean of  $2/3$  and  $1/3$  is (approx) 0.44444.

## $F_1$ Score - Examples

Consider the cancer example:

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Here  $F_1 = \frac{2TP}{2TP+FP+FN} = (2 \cdot 6)/((2 \cdot 6) + 1 + 2) = 0.8$ .

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Our imbalanced example:

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	Pos	Neg
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Here  $F_1 = \frac{2TP}{2TP+FP+FN} = (2 \cdot 1)/((2 \cdot 1) + 0 + 9) = 0.18$ .

Note that the average of Precision and Recall is 0.55, which would give us a much less severe warning that the classifier is bad.

## Imbalanced Classes Once More

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$$\text{Precision} = 90/99 \quad \text{Recall} = 90/90$$

$$F_1 = \frac{2TP}{2TP + FP + FN} = (2 \cdot 90)/(2 \cdot 90 + 9 + 0) = 0.95$$

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$$F_1 = \frac{2TP}{2TP + FP + FN} = (2 \cdot 90)/(2 \cdot 90 + 9 + 0) = 0.95$$

All great, except that the classifier sucks on the negative cases.

If you are concerned with the negative cases, swap the classes and compute another set of metrics.



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Works better with imbalanced classes.

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Works better with imbalanced classes.
- ▶ Criticised for giving Precision and Recall the same importance.
- ▶ Is not symmetric, ignores true negatives, i.e., is misleading for some cases of imbalanced classes.
- ▶ *Fowlkes-Mallows index* is a geometric mean of Precision and Recall (used in clustering).  
The geometric mean is between the arithmetic and harmonic mean. For example, the geometric mean of  $2/3$  and  $1/3$  is (approx) 0.4714.

## More Derived Metrics

<p>Positive predictive value (PPV), precision</p> $= \frac{TP}{PP} = 1 - FDR$	<p>False omission rate (FOR)</p> $= \frac{FN}{PN} = 1 - NPV$
<p>False discovery rate (FDR)</p> $= \frac{FP}{PP} = 1 - PPV$	<p>Negative predictive value (NPV)</p> $= \frac{TN}{PN} = 1 - FOR$

You can see that the negative predictive value becomes the Precision when we swap the classes (and vice versa).

## More Derived Metrics

<p>True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power</p> $= \frac{TP}{P} = 1 - FNR$	<p>False negative rate (FNR), miss rate</p> $= \frac{FN}{P} = 1 - TPR$
<p>False positive rate (FPR), probability of false alarm, fall-out</p> $= \frac{FP}{N} = 1 - TNR$	<p>True negative rate (TNR), specificity (SPC), selectivity</p> $= \frac{TN}{N} = 1 - FPR$

Note that *specificity* becomes Recall when we swap the classes (and vice versa).

For example, medical doctors communicate in terms of *sensitivity* and *specificity*.

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$$\text{TPR} = \text{Sensitivity} = \text{Recall} = \text{TP}/P = 6/8$$

How often is positive predicted positive?

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$$\text{TPR} = \text{Sensitivity} = \text{Recall} = \text{TP}/P = 6/8$$

How often is positive predicted positive?

$$\text{TNR} = \text{Specificity} = \text{TN}/N = 3/4$$

How often is negative predicted negative?



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Cancer	TP = 6	FN = 2
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Total	8 + 4 = 12	

$$\text{TPR} = \text{Sensitivity} = \text{Recall} = \text{TP}/P = 6/8$$

How often is positive predicted positive?

$$\text{TNR} = \text{Specificity} = \text{TN}/N = 3/4$$

How often is negative predicted negative?

$$\text{FPR} = \text{Prob. of false alarm} = \text{FP}/N = 1/4$$

How often is negative predicted positive?

Actual condition	Predicted condition	
	Cancer	Non-cancer
Cancer	TP = 6	FN = 2
Non-cancer	FP = 1	TN = 3
Total	8 + 4 = 12	

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How often is negative predicted negative?

$$\text{FPR} = \text{Prob. of false alarm} = \text{FP}/N = 1/4$$

How often is negative predicted positive?

$$\text{FNR} = \text{Miss rate} = \text{FN}/P = 2/8$$

How often is positive predicted negative?

# Evaluating Multi-class Classifiers

# Classification Into Multiple Classes

Assume classification into classes from a finite set  $C$ .

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How good are the predictions  $h_1, \dots, h_p$  w.r.t.  $c_1, \dots, c_p$ ?

There are many possible metrics ...

Consider an arbitrary (finite) number of classes in  $C$ .

## Confusion Matrix

Assume that  $C = \{1, \dots, m\}$ .



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Formally,

$$M_{ij} = |\{k \mid c_k = i \wedge h_k = j\}|$$

Actual	Predicted				
	1	...	$j$	...	$m$
1	$M_{11}$	...	$M_{1j}$	...	$M_{1m}$
$\vdots$	$\vdots$		$\vdots$		$\vdots$
$i$	$M_{i1}$	...	$M_{ij}$	...	$M_{im}$
$\vdots$	$\vdots$		$\vdots$		$\vdots$
$m$	$M_{m1}$	...	$M_{mj}$	...	$M_{mm}$

## Example

<b>Actual</b>	<b>Predicted</b>
big	big
big	big
small	big
medium	medium
big	small
big	big
small	small
small	small
medium	medium
medium	small
small	small
big	big
medium	small
small	medium
big	big

## Example

<b>Actual</b>	<b>Predicted</b>
big	big
big	big
small	big
medium	medium
big	small
big	big
small	small
small	small
medium	medium
medium	small
small	small
big	big
medium	small
small	medium
big	big

<b>Actual</b>	<b>Predicted</b>		
	<b>big</b>	<b>medium</b>	<b>small</b>
<b>big</b>	5	0	1
<b>medium</b>	0	2	2
<b>small</b>	1	1	3

Note that the diagonal counts the correctly classified samples.

The off-diagonal elements correspond to misclassified samples.

## Metrics

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For a given class  $i \in C$ :

$$\text{Precision}[i] = \frac{M_{ii}}{M_{\bullet i}} \quad \text{Recall}[i] = \frac{M_{ii}}{M_{i\bullet}}$$

$$F_1[i] = \frac{2 * \text{Precision}[i] * \text{Recall}[i]}{\text{Precision}[i] + \text{Recall}[i]}$$

Note that Precision, Recall, and  $F_1$  can be defined only for a given class!

## Example

Actual	Predicted		
	big	medium	small
big	5	0	1
medium	0	2	2
small	1	1	3

Compute the metrics.

## Example

$$\text{Accuracy} = (5+2+3)/15 = 0.66$$

$$\text{Precision}[\text{big}] = 5/6$$

$$\text{Precision}[\text{medium}] = 2/3$$

$$\text{Precision}[\text{small}] = 3/6$$

$$\text{Recall}[\text{big}] = 5/6$$

$$\text{Recall}[\text{medium}] = 2/4$$

$$\text{Recall}[\text{small}] = 3/5$$

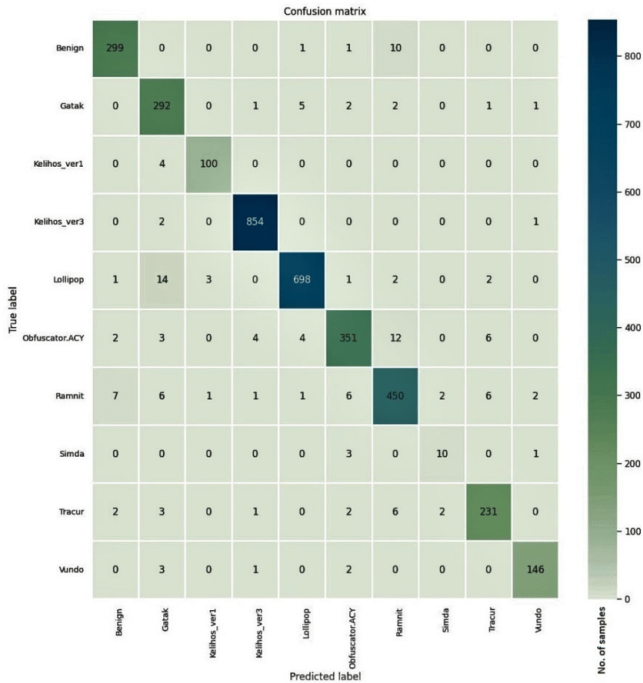
$$F_1[\text{big}] = \frac{2 * (5/6) * (5/6)}{(5/6) + (5/6)} = 5/6 = 0.83$$

$$F_1[\text{medium}] = 0.57$$

$$F_1[\text{small}] = 0.54$$

Actual	Predicted		
	big	medium	small
big	5	0	1
medium	0	2	2
small	1	1	3

How do you get a single number out of these? Average Precision, Recall, and  $F_1$  are usually computed, but one needs to be careful about the variance.





# Probabilistic Classifier Evaluation



# Binary Probabilistic Classifier

Assume binary classification into two classes  $\{0, 1\}$ .

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Consider a sequence of predictions generated by a classifier.

Now the classifier returns *probability of class 1* for a given input:

$$h_1, \dots, h_p \in [0, 1]$$

Here each  $h_k$  has been predicted for the  $k$ -th example  $(\vec{x}_k, c_k)$ .

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How to interpret the predictions  $h_1, \dots, h_p$ ?

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Let us fix predictions  $h_1, \dots, h_p$ .

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Given a threshold  $T \in [0, 1]$  we define

$$h_k^T = \begin{cases} 1 & \text{if } h_k \geq T \\ 0 & \text{if } h_k < T \end{cases}$$

For every  $T$  we can compute all the metrics (Precision, Recall, etc.)

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Given a metric MET and a threshold  $T$ , we denote by  $\text{MET}[T]$  the metric MET evaluated on  $h_1^T, \dots, h_p^T$ .



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We obtain

$$\text{TP}[T] = |\{k \mid h_k^T = 1 \wedge c_k = 1\}|$$

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and

TN[ $T$ ], FP[ $T$ ], FN[ $T$ ], Accuracy[ $T$ ], Precision[ $T$ ], Recall[ $T$ ],  $F_1$ [ $T$ ],  $\dots$

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and

$\text{TN}[T], \text{FP}[T], \text{FN}[T], \text{Accuracy}[T], \text{Precision}[T], \text{Recall}[T], F_1[T], \dots$

However, all metrics are now functions of the threshold  $T$ .

# Thresholded Classifier Metrics

<b>Index</b>	1	2	3	4	5	6	7	8	9	10	11	12
<b>Actual</b>	1	1	1	1	1	0	0	1	1	0	0	0
<b>Predicted</b>	.98	.95	.9	.86	.66	.48	.43	.42	.36	.15	.1	.05
T=0.5	TP	TP	TP	TP	TP	TN	TN	FN	FN	TN	TN	TN
T=0.42	TP	TP	TP	TP	TP	FP	FP	TP	FN	TN	TN	TN
T=0.1	TP	TP	TP	TP	TP	FP	FP	TP	TP	FP	FP	TN

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For example, consider  $T = 0.42$ , then

# Thresholded Classifier Metrics

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For example, consider  $T = 0.42$ , then

$$TP[T] = 6 \quad FP[T] = 2 \quad FN[T] = 1 \quad TN[T] = 3$$

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For example, consider  $T = 0.42$ , then

$$TP[T] = 6 \quad FP[T] = 2 \quad FN[T] = 1 \quad TN[T] = 3$$

$$Accuracy[T] = \frac{3+6}{12} \quad Precision[T] = \frac{6}{6+2} \quad Recall[T] = \frac{6}{6+1}$$

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$$Accuracy[T] = \frac{3+6}{12} \quad Precision[T] = \frac{6}{6+2} \quad Recall[T] = \frac{6}{6+1}$$

$$F_1[T] = \frac{2 \cdot 6/8 \cdot 6/7}{6/8 + 6/7} = 0.8$$



## Receiver Operating Characteristic (ROC)

Consider two metrics for a given  $T$ :

$$\text{TPR}[T] = \frac{\text{TP}[T]}{\text{P}[T]} \quad (\text{True Positive Rate})$$

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*ROC curve* is then a function  $\text{ROC} : [0, 1] \rightarrow [0, 1]^2$  defined by

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$$\text{ROC}(T) = (\text{TPR}[T], \text{FPR}[T])$$

Observe that

$$\text{ROC}(0) = (1, 1)$$

Because the classifier with  $T = 0$  simply classifies everything as positive, i.e., into the class 1.

Both  $\text{TPR}[T]$  and  $\text{FPR}[T]$  are non-increasing in  $T$ .

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►  $0.00 \leq T \leq 0.05$ :  $\text{TPR} = 1$  and  $\text{FPR} = 1$

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<b>Actual</b>	1	1	1	1	1	0	0	1	1	0	0	0
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Index	1	2	3	4	5	6	7	8	9	10	11	12
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- ▶  $0.36 < T \leq 0.42$ :  $\text{TPR} = 6/7$  and  $\text{FPR} = 2/5$

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<b>Actual</b>	1	1	1	1	1	0	0	1	1	0	0	0
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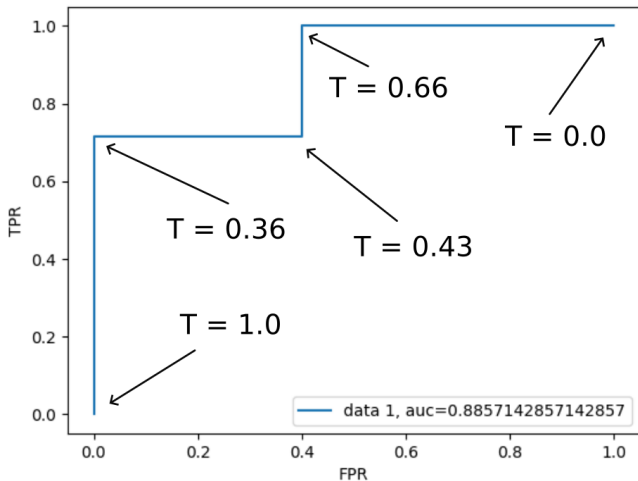
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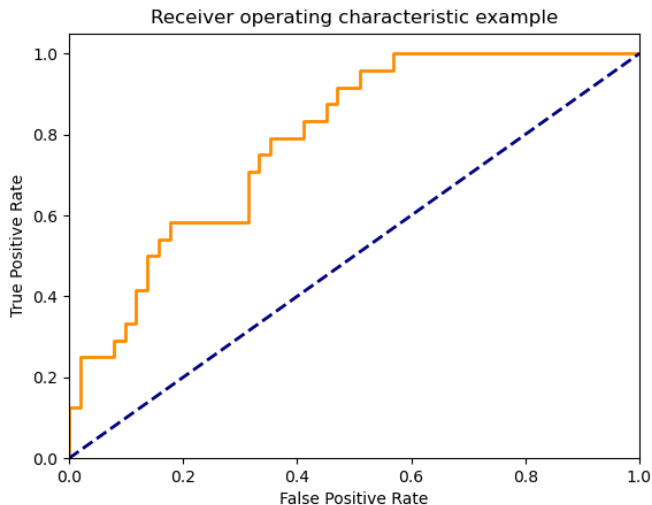
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# ROC

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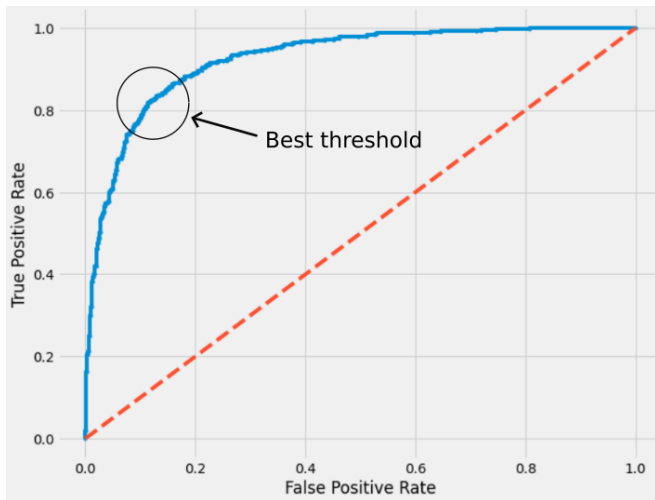


# Iris Dataset - A Classifier



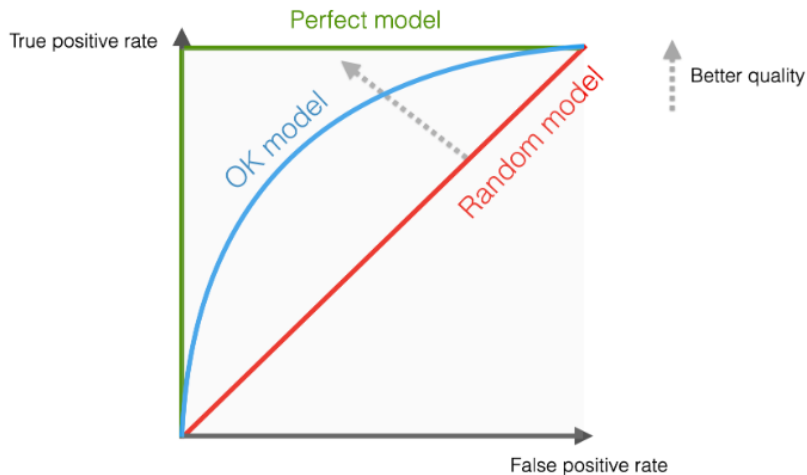
Example from the scikit-learn manual - SVM classifier trained in Iris

## Using ROC and Threshold



Search for the best threshold at the elbow of the ROC curve.

# ROC - Explanation

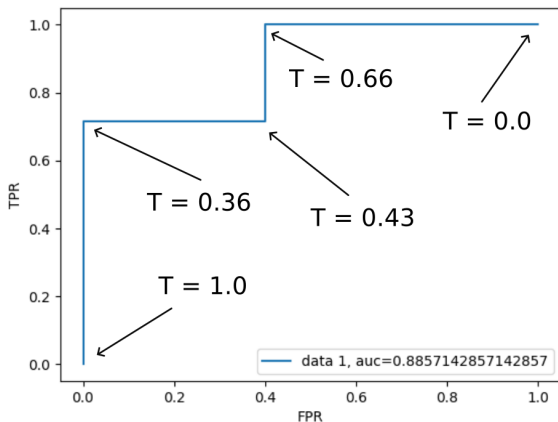


The larger the *area under the ROC curve (ROC-AUC)*, the better.

ROC-AUC ranges from 0 to 1.  $\text{ROC-AUC} \approx 0.5$  indicates random guessing.

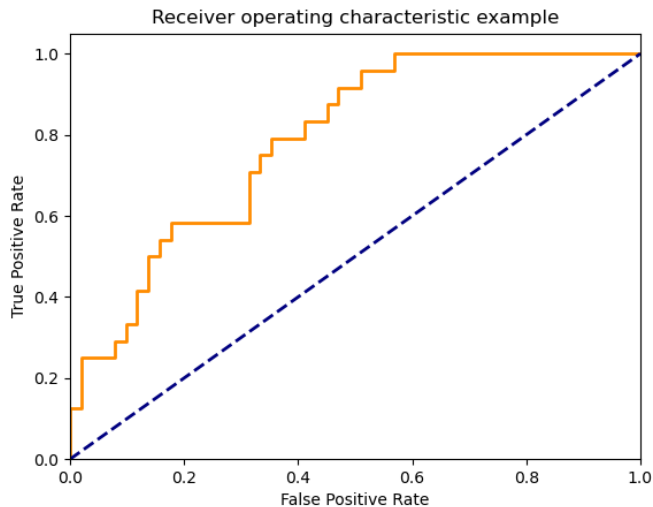
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ROC-AUC = 0.8857

# Iris - ROC-AUC



ROC-AUC = 0.79



# ROC-AUC - Probabilistic Interpretation

How is the ROC-AUC connected with the samples?

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The ROC-AUC is the probability of succeeding in the  $h_i > h_j$  test.

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There are still several questions unanswered:

- ▶ When to use the metrics.
- ▶ How to estimate the influence of sampling the dataset.

## Use of Evaluation Metrics

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- ▶ Hyperparameter fine-tuning.
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Keep in mind that the metrics are artificial, and the results of the model are roughly summarized.

It would be best if you always strived to test the proper functionality of your model in as natural conditions as possible.

For example, a model for medical diagnosis should be evaluated by medical doctors who may observe many features of its behavior that are difficult to express quantitatively.

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We will consider these issues in some later lecture. Concretely,

- ▶ *Bias-variance* tradeoff
- ▶ *Statistical tests* for testing
  - ▶ significance of the metrics values,
  - ▶ paired t-tests for comparing models.

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## *Thresholding*

- ▶ Introduce a threshold  $0 \leq t \leq 1$
- ▶ Demand, one of the two metrics (typically the Recall), to be at least  $t$ . That is

$$\text{Recall}_1 \geq t \quad \text{Recall}_2 \geq t$$

- ▶ Compare the values of the other metric numerically. In our case, decide whether

$$\text{Precision}_1 \geq \text{Precision}_2$$

(Still need to be concerned about the statistical significance.)

## Example

Actual condition	Predicted condition	
	Canc.	Non-canc.
Cancer	6	2
Non-canc.	1	3
Total	8 + 4 = 12	

Actual condition	Predicted condition	
	Canc.	Non-canc.
Cancer	5	3
Non-canc.	0	4
Total	8 + 4 = 12	

$$\text{Precision}_1 = \frac{6}{7} \quad \text{Recall}_1 = \frac{6}{8}$$

$$\text{Precision}_2 = \frac{5}{5} = 1 \quad \text{Recall}_2 = \frac{5}{8}$$

Consider a threshold  $t$  on the Recall.

The second classifier is better if the threshold  $t$  is  $5/8$ .

If the threshold  $t$  is  $6/8$ , then the second classifier is unacceptable.

# Linear Models

## Numerical features

- ▶ Throughout this lecture we assume that all features are numerical, i.e., feature vectors belong to  $\mathbb{R}^n$ .



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- ▶ Throughout this lecture we assume that all features are numerical, i.e., feature vectors belong to  $\mathbb{R}^n$ .
- ▶ Most non-numerical features can be conveniently transformed to numerical ones.

## For example:

- ▶ Colors  $\{blue, red, yellow\}$  can be represented by

$$\{(1, 0, 0), (0, 1, 0), (0, 0, 1)\}$$

(one-hot encoding)

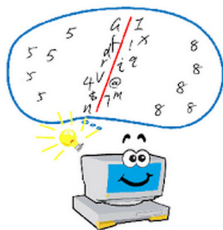
- ▶ Words can be embedded into vector spaces by various means (word2vec etc.)
- ▶ A black-and-white picture of  $x \times y$  pixels can be encoded as a vector of  $xy$  numbers that capture the shades of gray of the pixels.  
(Even though this is not the best way of representing images.)

# Basic Problems

We consider two basic problems:

- (Binary) classification

**Our goal:** Classify inputs into two categories.

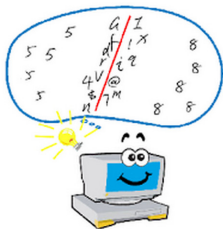


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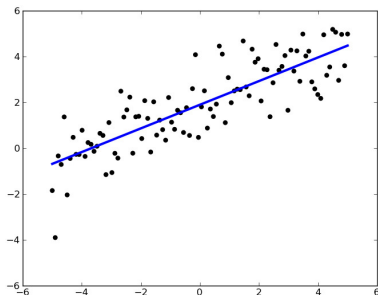
- (Binary) classification

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- Regression

**Our goal:** Find a (hypothesized) functional dependency in data.



# Linear Models

## Binary Classification

# Binary classification in $\mathbb{R}^n$

## Our goal:

- ▶ Given a set  $D$  of training examples of the form  $(\vec{x}, c)$  where  $\vec{x} \in \mathbb{R}^n$  and  $c \in \{0, 1\}$ ,

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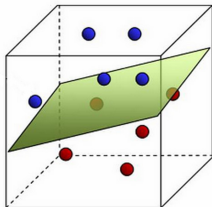
## Comments:

- ▶ In practice, we often do not strictly demand  $h(\vec{x}) = c$  for all training examples  $(\vec{x}, c) \in D$  (often it is impossible)
- ▶ We are more interested in good **generalization**, that is how well  $h$  classifies new instances that do not belong to  $D$ .  
(Recall that we usually evaluate accuracy of the resulting hypothesized function  $h$  on a test set.)

# Models

We consider two kinds of models:

- ▶ Linear (affine) classifiers (this lecture)

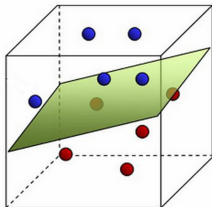




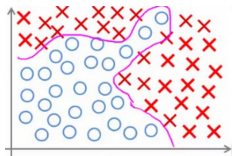
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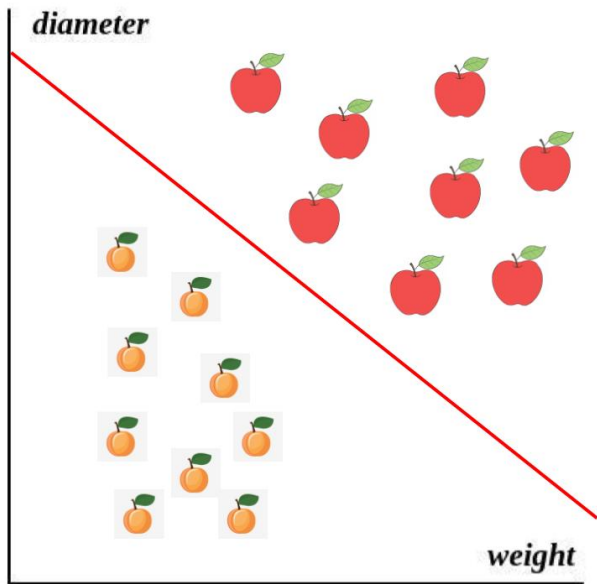
- ▶ Linear (affine) classifiers (this lecture)



- ▶ Non-linear classifiers (kernel SVM, neural networks) (later lectures)



## Linear Classifier – Example



# Length and Scalar Product of Vectors

- ▶ We consider vectors  $\vec{x} = (x_1, \dots, x_n) \in \mathbb{R}^m$ .

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The distance between two vectors (points)  $\vec{x}, \vec{y}$  is  $||\vec{x} - \vec{y}||$ .
- ▶ *Scalar product*  $\vec{x} \cdot \vec{y}$  of vectors  $\vec{x} = (x_1, \dots, x_n)$  and  $\vec{y} = (y_1, \dots, y_n)$  defined by

$$\vec{x} \cdot \vec{y} = \sum_{i=1}^n x_i y_i$$

- ▶ Recall that  $\vec{x} \cdot \vec{y} = ||\vec{x}|| ||\vec{y}|| \cos \theta$  where  $\theta$  is the angle between  $\vec{x}$  and  $\vec{y}$ . That is  $\vec{x} \cdot \vec{y}$  is the length of the projection of  $\vec{y}$  on  $\vec{x}$  multiplied by  $||\vec{x}||$ .
- ▶ Note that  $\vec{x} \cdot \vec{x} = ||\vec{x}||^2$

# Linear Classifier

A *linear classifier*  $h[\vec{w}]$  is determined by a vector of *weights*  $\vec{w} = (w_0, w_1, \dots, w_n) \in \mathbb{R}^{n+1}$  as follows:

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$$h[\vec{w}](\vec{x}) := \begin{cases} 1 & w_0 + \sum_{i=1}^n w_i \cdot x_i \geq 0 \\ 0 & w_0 + \sum_{i=1}^n w_i \cdot x_i < 0 \end{cases}$$

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More succinctly:

$$h(\vec{x}) = \operatorname{sgn} \left( w_0 + \sum_{i=1}^n w_i \cdot x_i \right) \quad \text{where} \quad \operatorname{sgn}(y) = \begin{cases} 1 & y \geq 0 \\ 0 & y < 0 \end{cases}$$

We define *separating hyperplane* determined by  $\vec{w}$  as the set of all  $\vec{x} \in \mathbb{R}^n$  satisfying  $w_0 + \sum_{i=1}^n w_i \cdot x_i = 0$ .



$$w_0 + w_1x_1 + w_2x_2 = 0$$

$$w_0 = -3$$

$$w_1 = 2$$

$$w_2 = 1$$

$$w_0 + w_1x_1 + w_2x_2 > 0$$

$$(w_1, w_2) = (2, 1)$$

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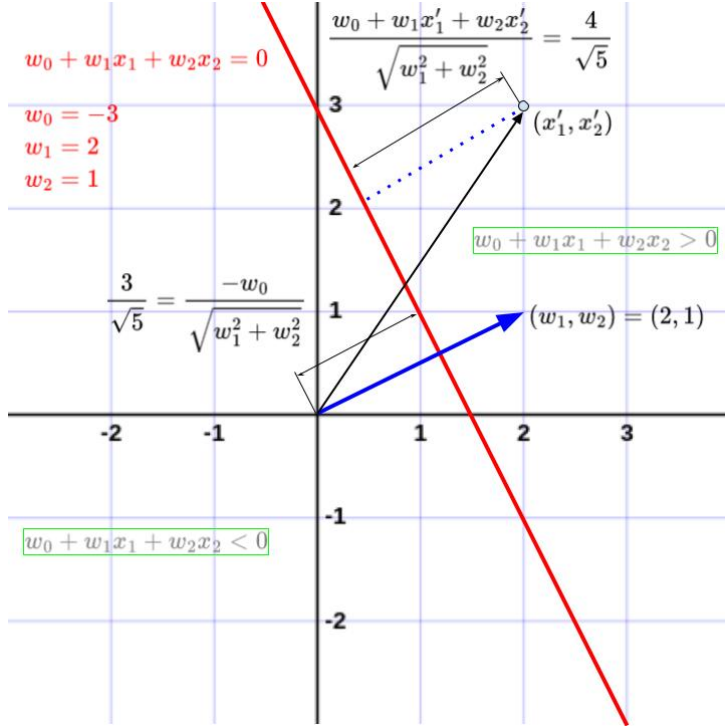
$$w_2 = 1$$

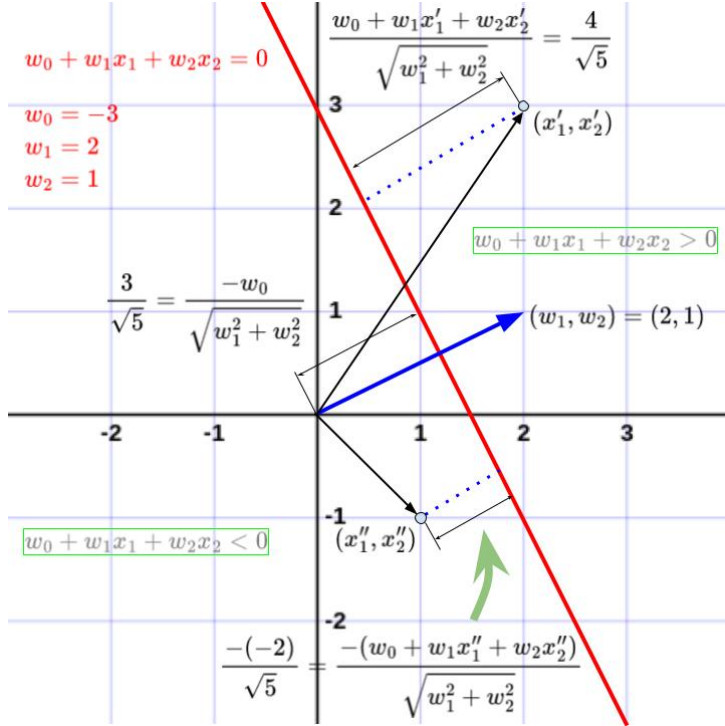
$$\frac{3}{\sqrt{5}} = \frac{-w_0}{\sqrt{w_1^2 + w_2^2}}$$

$$w_0 + w_1x_1 + w_2x_2 > 0$$

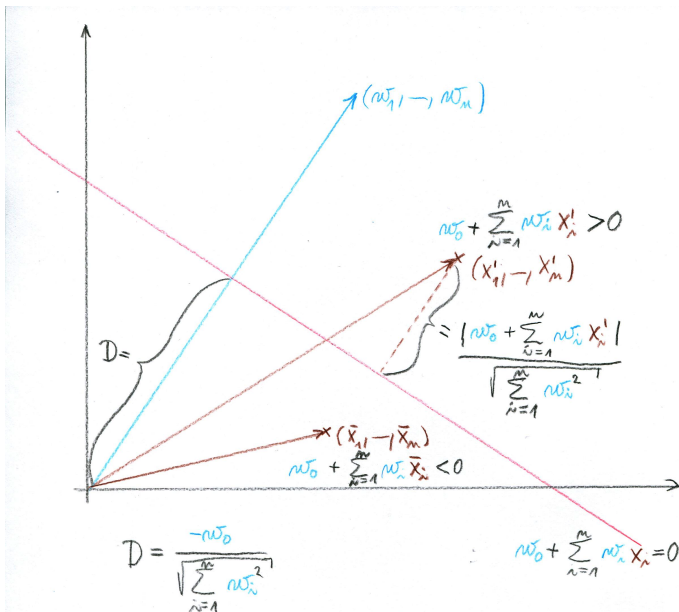
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# Linear Classifier – Geometry



## Linear Classifier – Notation

Given  $\vec{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$  we define an *augmented feature vector*

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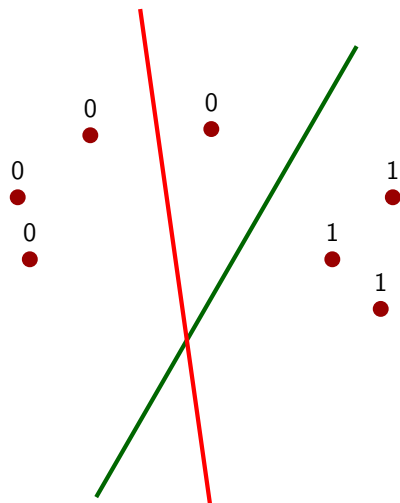
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This makes the notation for the linear classifier more succinct:

$$h[\vec{w}](\vec{x}) = \text{sgn}(\vec{w} \cdot \tilde{\mathbf{x}})$$

# Linear Classifier – Learning



- ▶ classification in the plane using a linear classifier
- ▶ if a point is incorrectly classified, the learning algorithm turns the line (hyperplane) to improve the classification



# Perceptron Learning

- ▶ Given a training set

$$D = \{(\vec{x}_1, c_1), (\vec{x}_2, c_2), \dots, (\vec{x}_p, c_p)\}$$

Here  $\vec{x}_k = (x_{k1}, \dots, x_{kn}) \in \mathbb{R}^n$  and  $c_k \in \{0, 1\}$ .

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$D$  is **linearly separable** if there is a vector  $\vec{w} \in \mathbb{R}^{n+1}$  which is consistent with  $D$ .

- ▶ Our goal is to find a consistent  $\vec{w}$  assuming that  $D$  is linearly separable.

# Perceptron – Learning Algorithm

## Online learning algorithm:

Idea: Cyclically go through the training examples in  $D$  and adapt weights.

Whenever an example is incorrectly classified, turn the hyperplane so that the example becomes closer to its correct half-space.

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Here  $k = (t \bmod p) + 1$ , i.e., the examples are considered cyclically, and  $0 < \varepsilon \leq 1$  is a **learning rate**.

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## Theorem (Rosenblatt)

*If  $D$  is linearly separable, then there is  $t^*$  such that  $\vec{w}^{(t^*)}$  is consistent with  $D$ .*

## Example

Training set:

$$D = \{((2, -1), 1), ((2, 1), 1), ((1, 3), 0)\}$$

That is

$$\vec{x}_1 = (2, -1)$$

$$\tilde{\mathbf{x}}_1 = (\mathbf{1}, 2, -1)$$

$$\vec{x}_2 = (2, 1)$$

$$\tilde{\mathbf{x}}_2 = (\mathbf{1}, 2, 1)$$

$$\vec{x}_3 = (1, 3)$$

$$\tilde{\mathbf{x}}_3 = (\mathbf{1}, 1, 3)$$

$$c_1 = 1$$

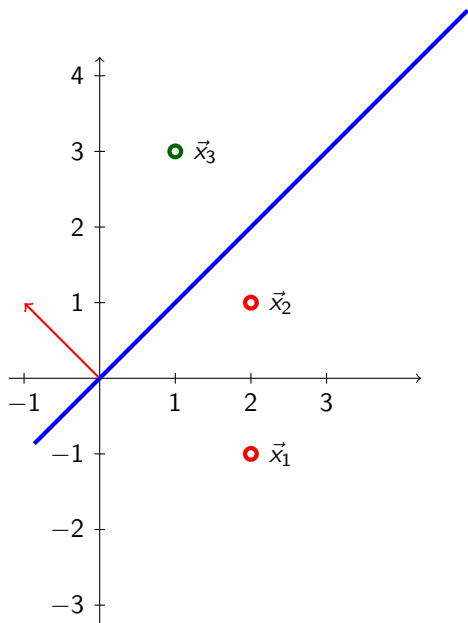
$$c_2 = 1$$

$$c_3 = 0$$

Assume that the initial vector  $\vec{w}^{(0)}$  is  $\vec{w}^{(0)} = (0, -1, 1)$ .

Consider  $\varepsilon = 1$ .

## Example: Separating by $\vec{w}^{(0)}$



Denoting  $\vec{w}^{(0)} = (w_0, w_1, w_2) = (0, -1, 1)$  the blue separating line is given by  $w_0 + w_1x_1 + w_2x_2 = 0$ .

The red vector normal to the blue line is  $(w_1, w_2)$ .

The points on the side of  $(w_1, w_2)$  are assigned 1 by the classifier, the others zero. (In this case  $\vec{x}_3$  is assigned one and  $\vec{x}_1, \vec{x}_2$  are assigned zero, all of this is inconsistent with  $c_1 = 1, c_2 = 1, c_3 = 0$ .)

## Example: Computing $\vec{w}^{(1)}$

We have

$$\vec{w}^{(0)} \cdot \tilde{\mathbf{x}}_1 = (0, -1, 1) \cdot (1, 2, -1) = 0 - 2 - 1 = -3$$

thus

$$\text{sgn} \left( \vec{w}^{(0)} \cdot \tilde{\mathbf{x}}_1 \right) = 0$$

and thus

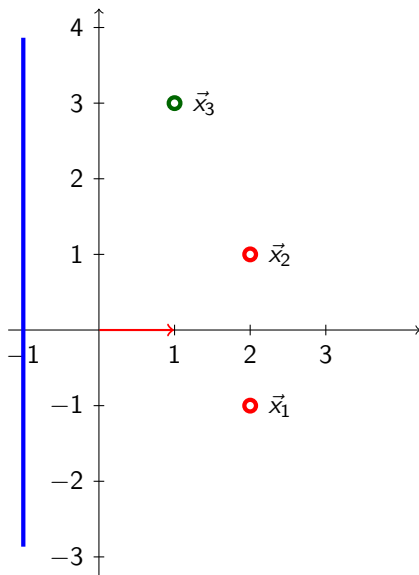
$$\text{sgn} \left( \vec{w}^{(0)} \cdot \tilde{\mathbf{x}}_1 \right) - c_1 = 0 - 1 = -1$$

(I.e.,  $\tilde{\mathbf{x}}_1$  is not correctly classified, and  $\vec{w}^{(0)}$  is not consistent with  $D$ .)

Hence,

$$\begin{aligned} \vec{w}^{(1)} &= \vec{w}^{(0)} - \left( \text{sgn} \left( \vec{w}^{(0)} \cdot \tilde{\mathbf{x}}_1 \right) - c_1 \right) \cdot \tilde{\mathbf{x}}_1 \\ &= \vec{w}^{(0)} + \tilde{\mathbf{x}}_1 \\ &= (0, -1, 1) + (1, 2, -1) \\ &= (1, 1, 0) \end{aligned}$$

Example: Separating by  $\vec{w}^{(1)}$



## Example: Computing $\vec{w}^{(2)}$

We have

$$\vec{w}^{(1)} \cdot \tilde{\mathbf{x}}_2 = (1, 1, 0) \cdot (1, 2, 1) = 1 + 2 = 3$$

thus

$$\text{sgn} \left( \vec{w}^{(1)} \cdot \tilde{\mathbf{x}}_2 \right) = 1$$

and thus

$$\text{sgn} \left( \vec{w}^{(1)} \cdot \tilde{\mathbf{x}}_2 \right) - c_2 = 1 - 1 = 0$$

(I.e.,  $\vec{x}_2$  is currently correctly classified by  $\vec{w}^{(1)}$ . However, as we will see,  $\vec{x}_3$  is not well classified.)

Hence,

$$\vec{w}^{(2)} = \vec{w}^{(1)} = (1, 1, 0)$$



## Example: Computing $\vec{w}^{(3)}$

We have

$$\vec{w}^{(2)} \cdot \tilde{\mathbf{x}}_3 = (1, 1, 0) \cdot (1, 1, 3) = 1 + 1 = 2$$

thus

$$\text{sgn} \left( \vec{w}^{(2)} \cdot \tilde{\mathbf{x}}_3 \right) = 1$$

and thus

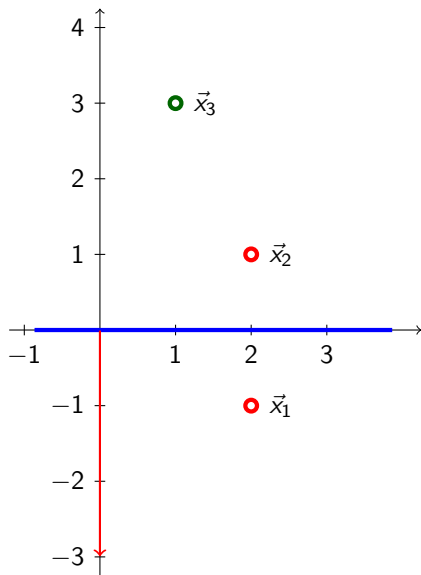
$$\text{sgn} \left( \vec{w}^{(2)} \cdot \tilde{\mathbf{x}}_3 \right) - c_3 = 1 - 0 = 1$$

(This means that  $\tilde{\mathbf{x}}_3$  is not well classified, and  $\vec{w}^{(2)}$  is not consistent with  $D$ .)

Hence,

$$\begin{aligned} \vec{w}^{(3)} &= \vec{w}^{(2)} - \left( \text{sgn} \left( \vec{w}^{(2)} \cdot \tilde{\mathbf{x}}_3 \right) - c_3 \right) \cdot \tilde{\mathbf{x}}_3 \\ &= \vec{w}^{(2)} - \tilde{\mathbf{x}}_3 \\ &= (1, 1, 0) - (1, 1, 3) \\ &= (0, 0, -3) \end{aligned}$$

Example: Separating by  $\vec{w}^{(3)}$



## Example: Computing $\vec{w}^{(4)}$

We have

$$\vec{w}^{(3)} \cdot \tilde{\mathbf{x}}_1 = (0, 0, -3) \cdot (1, 2, -1) = 3$$

thus

$$\text{sgn}(\vec{w}^{(3)} \cdot \tilde{\mathbf{x}}_1) = 1$$

and thus

$$\text{sgn}(\vec{w}^{(3)} \cdot \tilde{\mathbf{x}}_1) - c_1 = 1 - 1 = 0$$

(I.e.,  $\vec{x}_1$  is currently correctly classified by  $\vec{w}^{(3)}$ . However, we shall see that  $\vec{x}_2$  is not.)

Hence,

$$\vec{w}^{(4)} = \vec{w}^{(3)} = (0, 0, -3)$$

## Example: Computing $\vec{w}^{(5)}$

We have

$$\vec{w}^{(4)} \cdot \tilde{\mathbf{x}}_2 = (0, 0, -3) \cdot (1, 2, 1) = -3$$

thus

$$\text{sgn}(\vec{w}^{(4)} \cdot \tilde{\mathbf{x}}_2) = 0$$

and thus

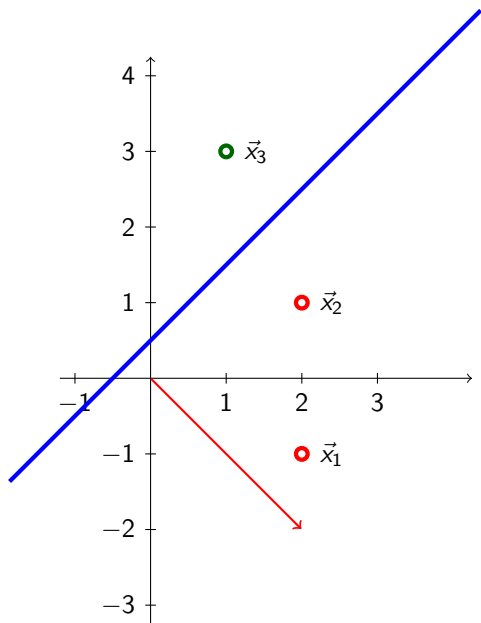
$$\text{sgn}(\vec{w}^{(4)} \cdot \tilde{\mathbf{x}}_2) - c_2 = 0 - 1 = -1$$

(I.e.,  $\tilde{\mathbf{x}}_2$  is not correctly classified, and  $\vec{w}^{(4)}$  is not consistent with  $D$ .)

Hence,

$$\begin{aligned}\vec{w}^{(5)} &= \vec{w}^{(4)} - \left( \text{sgn}(\vec{w}^{(4)} \cdot \tilde{\mathbf{x}}_2) - c_2 \right) \cdot \tilde{\mathbf{x}}_2 \\ &= \vec{w}^{(4)} + \tilde{\mathbf{x}}_2 \\ &= (0, 0, -3) + (1, 2, 1) \\ &= (1, 2, -2)\end{aligned}$$

Example: Separating by  $\vec{w}^{(5)}$



## Example: The result

The vector  $\vec{w}^{(5)}$  is consistent with  $D$ :

$$\operatorname{sgn}\left(\vec{w}^{(5)} \cdot \tilde{\mathbf{x}}_1\right) = \operatorname{sgn}\left((1, 2, -2) \cdot (1, 2, -1)\right) = \operatorname{sgn}(7) = 1 = c_1$$

$$\operatorname{sgn}\left(\vec{w}^{(5)} \cdot \tilde{\mathbf{x}}_2\right) = \operatorname{sgn}\left((1, 2, -2) \cdot (1, 2, 1)\right) = \operatorname{sgn}(3) = 1 = c_2$$

$$\operatorname{sgn}\left(\vec{w}^{(5)} \cdot \tilde{\mathbf{x}}_3\right) = \operatorname{sgn}\left((1, 2, -2) \cdot (1, 1, 3)\right) = \operatorname{sgn}(-3) = 0 = c_3$$

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Compute a sequence of weight vectors  $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \dots$

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Here  $0 < \varepsilon \leq 1$  is a **learning rate**.

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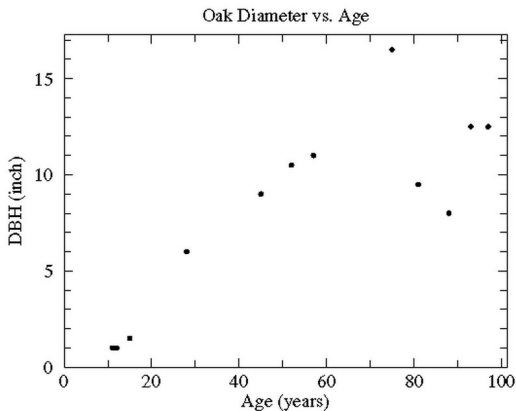
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# Linear Regression

# Linear Regression – Oaks in Wisconsin

This example is from *How to Lie with Statistics* by Darrell Huff (1954)

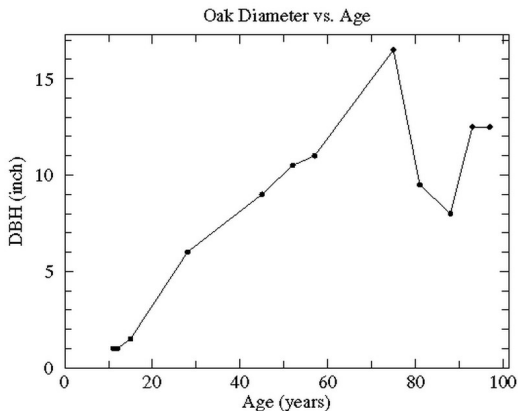
Age (years)	DBH (inch)
97	12.5
93	12.5
88	8.0
81	9.5
75	16.5
57	11.0
52	10.5
45	9.0
28	6.0
15	1.5
12	1.0
11	1.0



# Linear Regression – Oaks in Wisconsin

This example is from *How to Lie with Statistics* by Darrell Huff (1954)

Age (years)	DBH (inch)
97	12.5
93	12.5
88	8.0
81	9.5
75	16.5
57	11.0
52	10.5
45	9.0
28	6.0
15	1.5
12	1.0
11	1.0

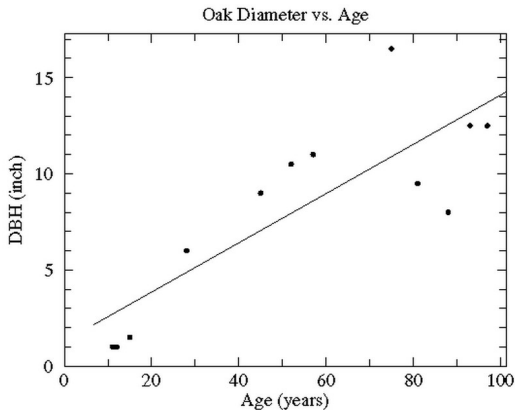


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possibly **YES!**

# Linear Regression

## Our goal:

- ▶ Given a set  $D$  of training examples of the form  $(\vec{x}, f)$  where  $\vec{x} \in \mathbb{R}^n$  and  $f \in \mathbb{R}$ ,

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Here  $\approx$  means that the values are somewhat close to each other w.r.t. an appropriate *error function*  $E$ .

Also called *loss function*.



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In what follows we use the *squared error* defined by

$$E = \frac{1}{2} \sum_{(\vec{x}, f) \in D} (h(\vec{x}) - f)^2$$

Our goal is to minimize  $E$ .

The main reason is that this function has nice mathematical properties (as opposed, e.g., to  $\sum_{(\vec{x}, f) \in D} |h(\vec{x}) - f|$ ).

# Linear Function Approximation

- ▶ Given a set  $D$  of training examples:

$$D = \{(\vec{x}_1, f_1), (\vec{x}_2, f_2), \dots, (\vec{x}_p, f_p)\}$$

Here  $\vec{x}_k = (x_{k1}, \dots, x_{kn}) \in \mathbb{R}^n$  and  $f_k \in \mathbb{R}$ .

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Recall that  $\tilde{\mathbf{x}}_k = (x_{k0}, x_{k1} \dots, x_{kn})$  where  $x_{k0} = 1$ .

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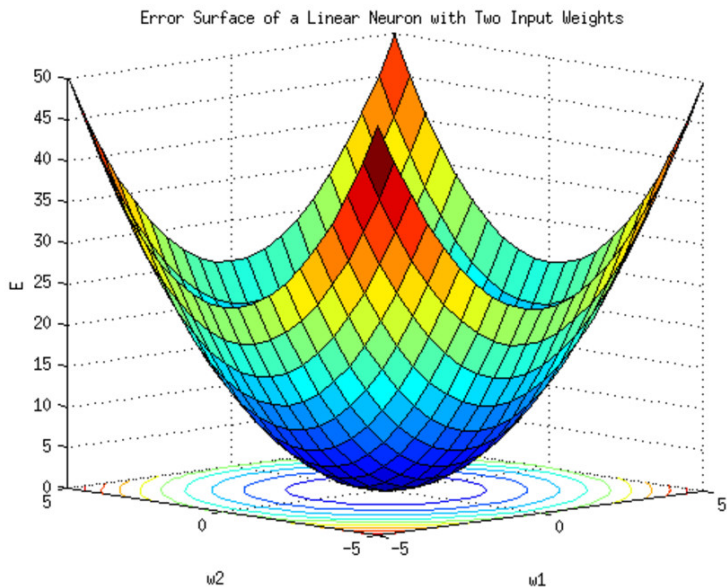
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- ▶ **Squared Error Function:**

$$E(\vec{w}) = \frac{1}{2} \sum_{k=1}^p (\vec{w} \cdot \tilde{\mathbf{x}}_k - f_k)^2 = \frac{1}{2} \sum_{k=1}^p \left( \sum_{i=0}^n w_i x_{ki} - f_k \right)^2$$

# Error function



## Gradient of the Error Function

Consider the **gradient** of the error function:

$$\nabla E(\vec{w}) = \left( \frac{\partial E}{\partial w_0}(\vec{w}), \dots, \frac{\partial E}{\partial w_n}(\vec{w}) \right) = \sum_{k=1}^p (\vec{w} \cdot \tilde{\mathbf{x}}_k - f_k) \cdot \tilde{\mathbf{x}}_k$$

What is the gradient  $\nabla E(\vec{w})$ ? It is a vector in  $\mathbb{R}^{n+1}$  which points in the direction of the steepest *ascent* of  $E$  (its length corresponds to the steepness). Note that here the vectors  $\tilde{\mathbf{x}}_k$  are *fixed* parameters of  $E$ !

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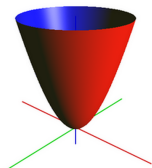
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**Fact:**

If  $\nabla E(\vec{w}) = \vec{0} = (0, \dots, 0)$ , then  $\vec{w}$  is a global minimum of  $E$ .

This follows from the fact that  $E$  is a convex paraboloid that has a unique extreme, which is a minimum.



## Gradient of the error function

Consider  $n = 1$ , which means that  $\vec{w} = (w_0, w_1)$  and we write  $x$  instead of  $\vec{x}$  since  $\vec{x} \in \mathbb{R}^n = \mathbb{R}^1 = \mathbb{R}$ .

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Consider a concrete training set:

$$\begin{aligned}\mathcal{T} &= \{(2, 1), (3, 2), (4, 5)\} \\ &= \{(x_1, f_1), (x_2, f_2), (x_3, f_3)\}\end{aligned}$$

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- ▶ In  $(t + 1)$ -th step,  $\vec{w}^{(t+1)}$  is computed as follows:

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Here  $0 < \varepsilon \leq 1$  is a learning rate.

Note that the algorithm is almost similar to the batch perceptron algorithm!

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## Proposition

*For sufficiently small  $\varepsilon > 0$  the sequence  $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \dots$  converges (component-wisely) to the global minimum of  $E$ .*

Training set:

$$D = \{(x_1, f_1), (x_2, f_2), (x_3, f_3)\} = \{(0, 0), (2, 1), (2, 2)\}$$

Note that input vectors are one dimensional, so we write them as numbers.

That is

$$x_1 = 0$$

$$x_2 = 2$$

$$x_3 = 2$$

$$\tilde{\mathbf{x}}_1 = (\mathbf{1}, 0)$$

$$\tilde{\mathbf{x}}_2 = (\mathbf{1}, 2)$$

$$\tilde{\mathbf{x}}_3 = (\mathbf{1}, 2)$$

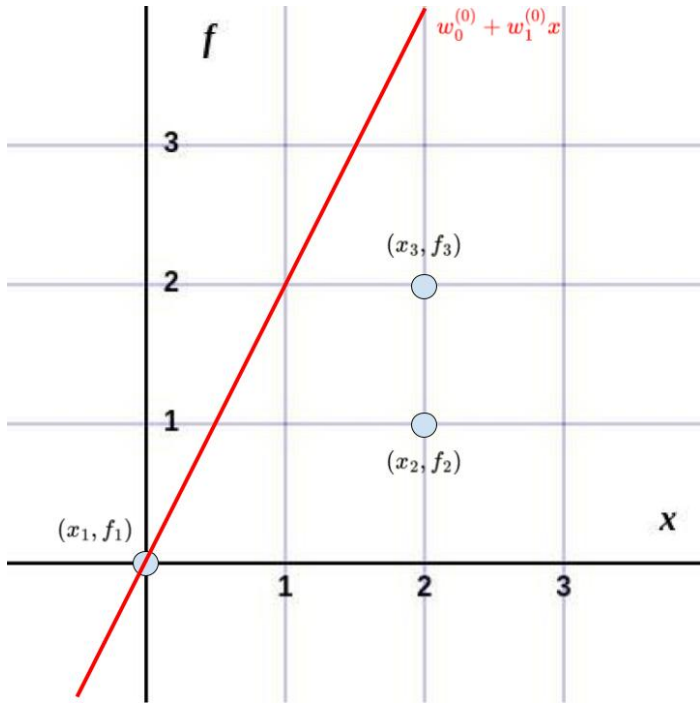
$$f_1 = 0$$

$$f_2 = 1$$

$$f_3 = 2$$

Assume that the initial vector  $\vec{w}^{(0)}$  is  $\vec{w}^{(0)} = (w_0^{(0)}, w_1^{(0)}) = (0, 2)$ .

Consider  $\varepsilon = \frac{1}{10}$ .



Training set:

$D = \{(x_1, f_1), (x_2, f_2), (x_3, f_3)\} = \{(0, 0), (2, 1), (2, 2)\}$  Augmented input vectors:  $\tilde{\mathbf{x}}_1 = (1, 0)$ ,  $\tilde{\mathbf{x}}_2 = (1, 2)$ ,  $\tilde{\mathbf{x}}_3 = (1, 2)$

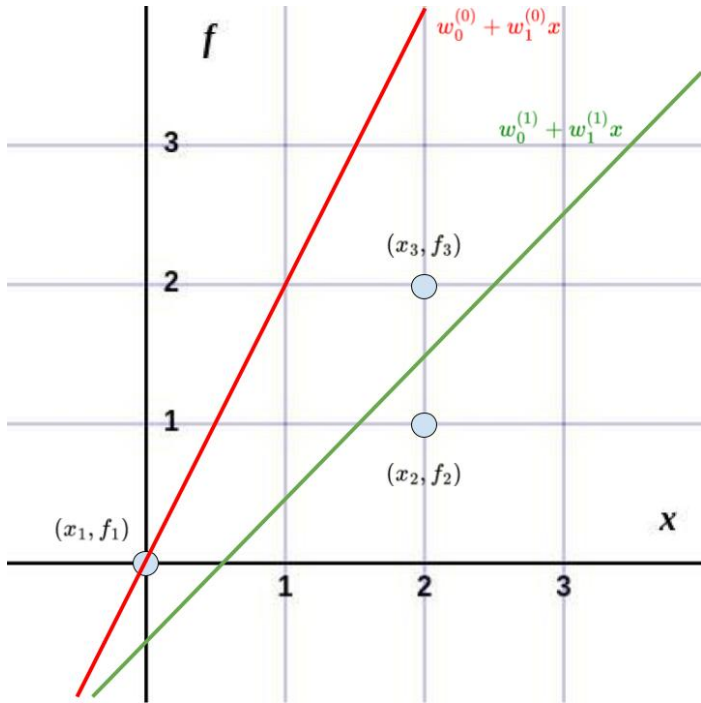
$$\begin{aligned}\nabla E(\vec{w}) &= \left( \frac{\partial E}{\partial w_0}(\vec{w}), \frac{\partial E}{\partial w_1}(\vec{w}) \right) = (w_0 + w_1 \cdot x_1 - f_1) \cdot \tilde{\mathbf{x}}_1 \\ &\quad + (w_0 + w_1 \cdot x_2 - f_2) \cdot \tilde{\mathbf{x}}_2 \\ &\quad + (w_0 + w_1 \cdot x_3 - f_3) \cdot \tilde{\mathbf{x}}_3\end{aligned}$$

For  $\vec{w}^{(0)} = (0, 2)$  we have

$$\begin{aligned}\nabla E(\vec{w}^{(0)}) &= (0 + 2 \cdot 0 - 0) \cdot (1, 0) \\ &\quad + (0 + 2 \cdot 2 - 1) \cdot (1, 2) \\ &\quad + (0 + 2 \cdot 2 - 2) \cdot (1, 2) = (3, 6) + (2, 4) = (5, 10)\end{aligned}$$

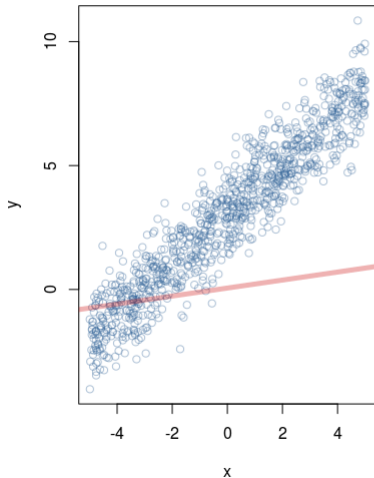
Finally,  $\vec{w}^{(1)}$  is computed by

$$\vec{w}^{(1)} = \vec{w}^{(0)} - \varepsilon \cdot \nabla E(\vec{w}^{(0)}) = (0, 2) - \frac{1}{10} \cdot (5, 10) = (-1/2, 1)$$

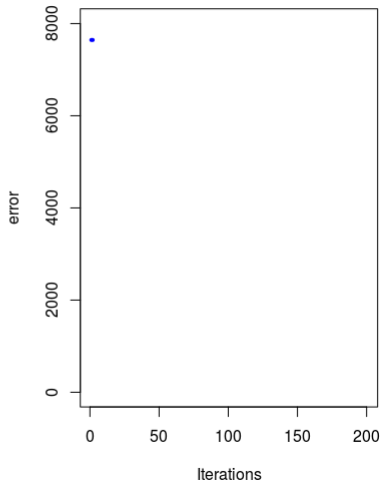


# Linear Regression - Animation

Linear regression by gradient descent



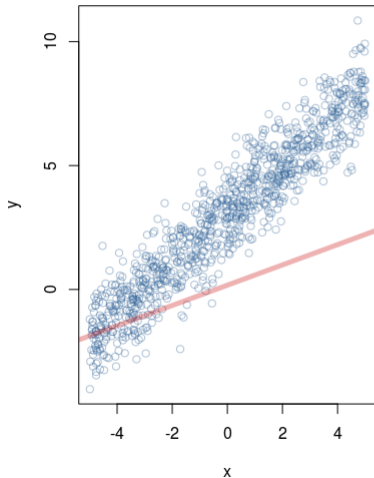
Error function



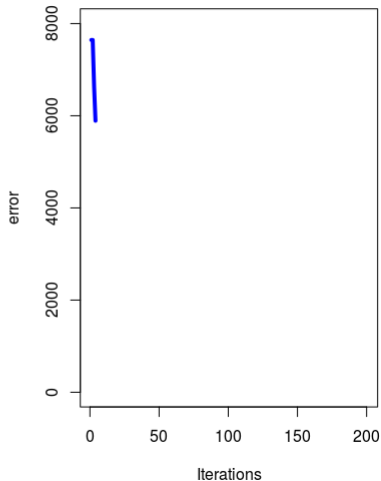


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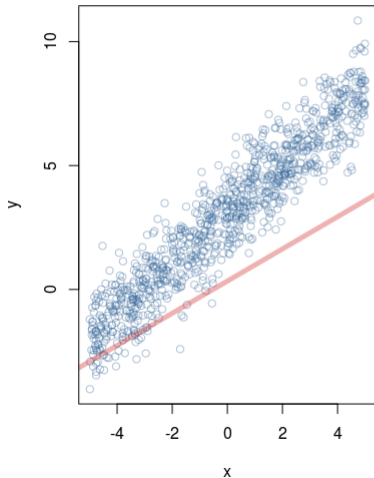


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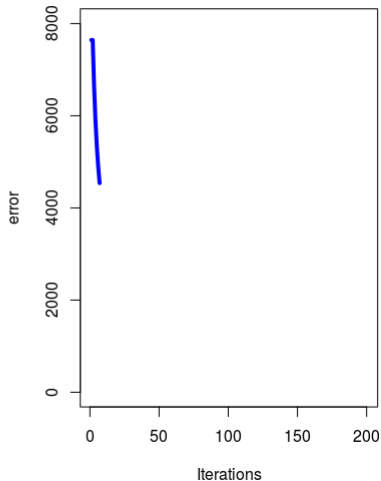


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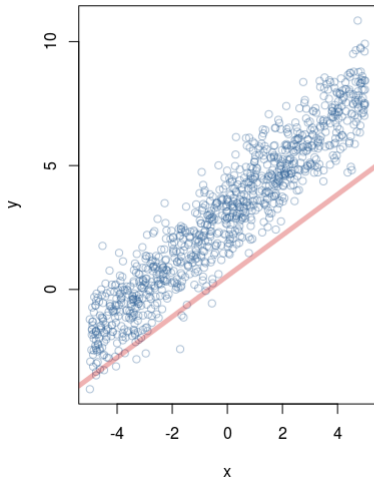


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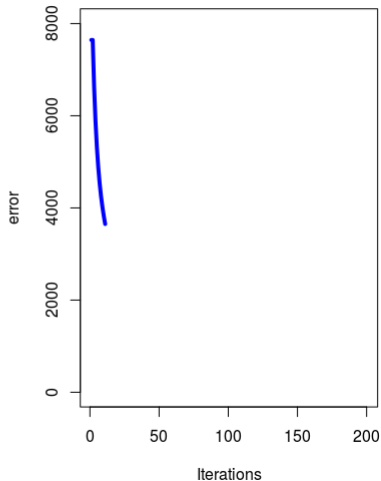


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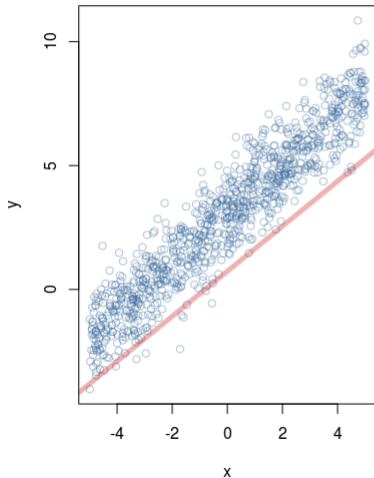


Error function

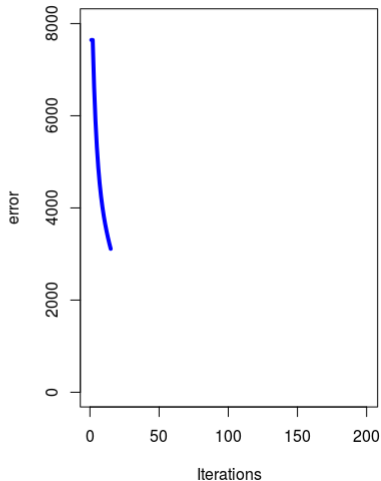


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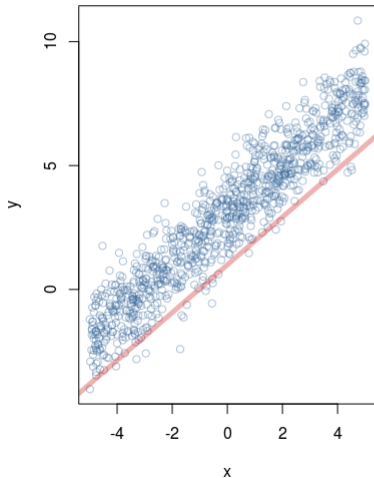


Error function

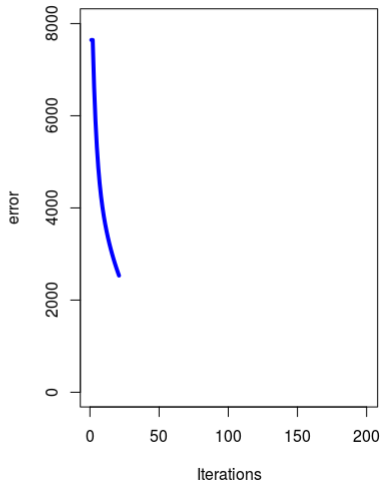


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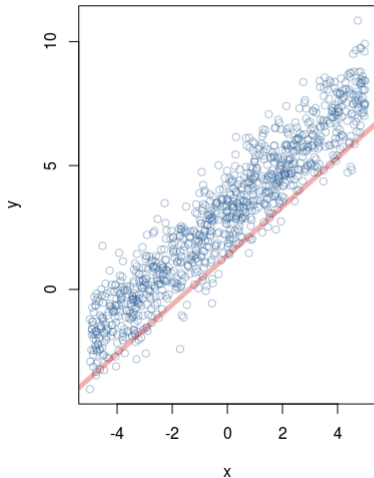


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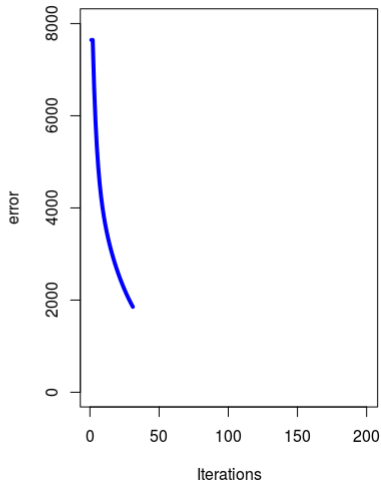


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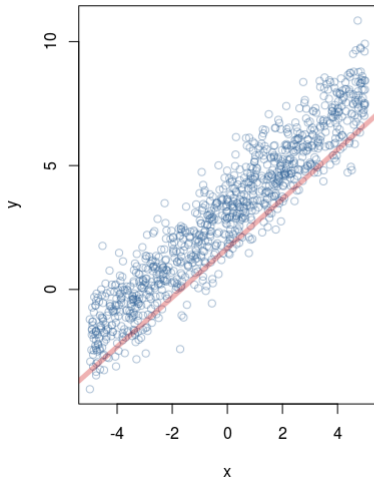


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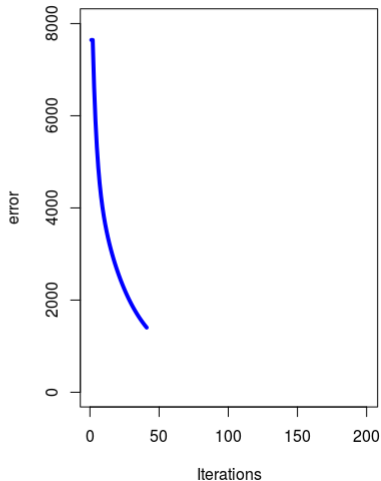


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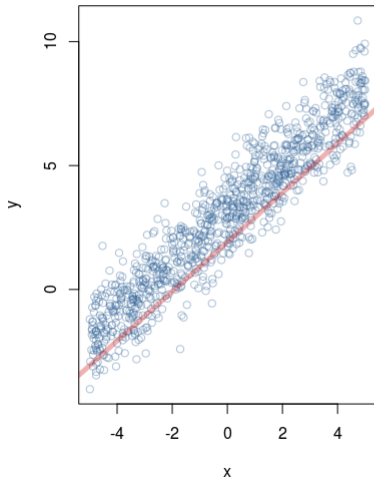


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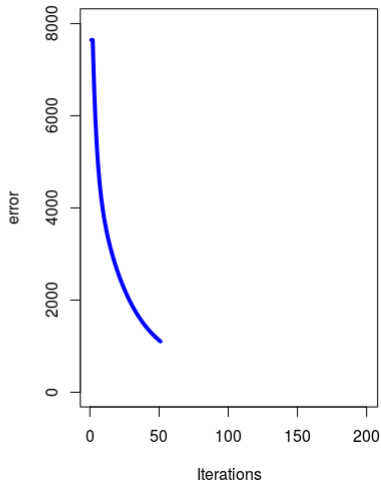


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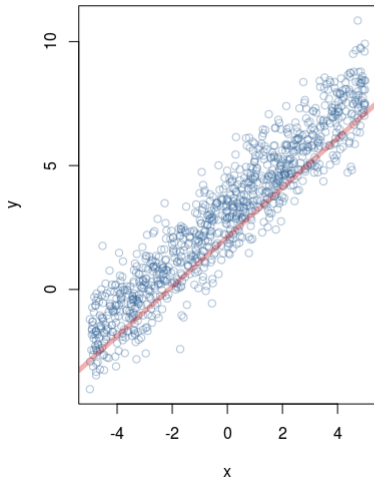
Error function



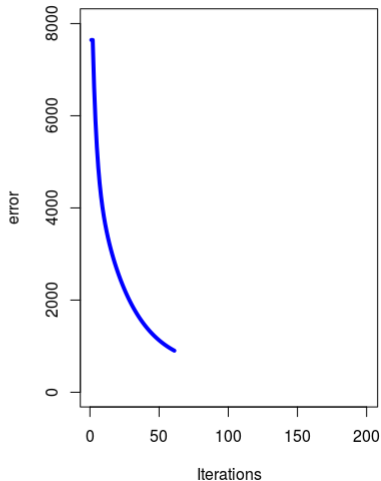


# Linear Regression - Animation

Linear regression by gradient descent

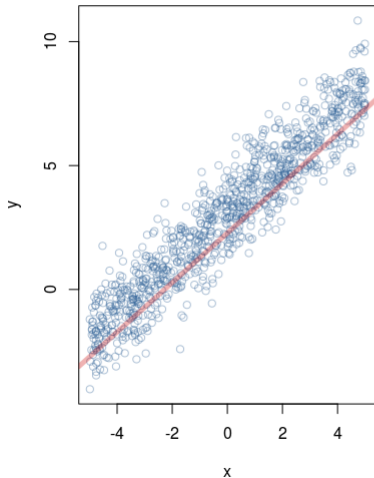


Error function

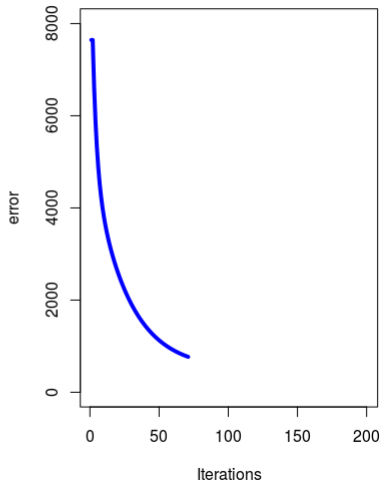


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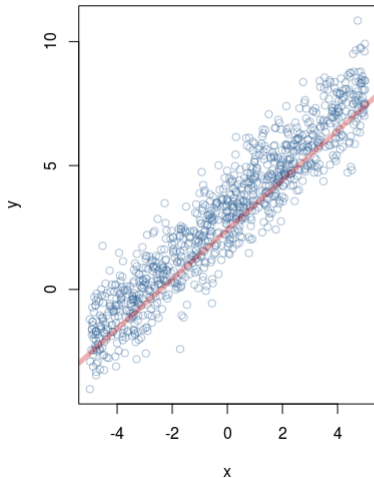


Error function

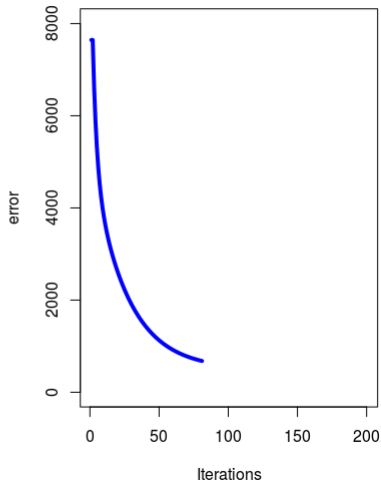


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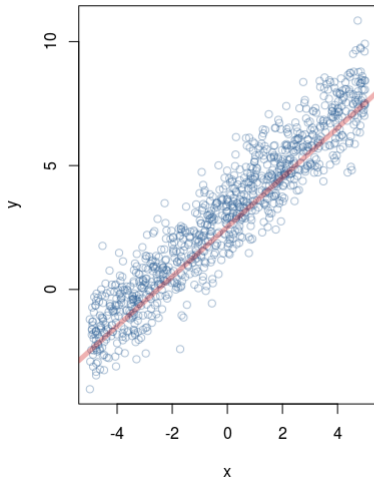


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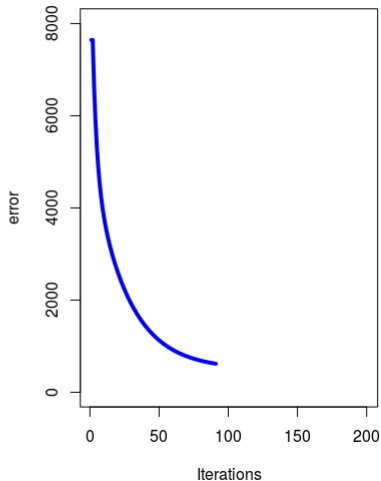


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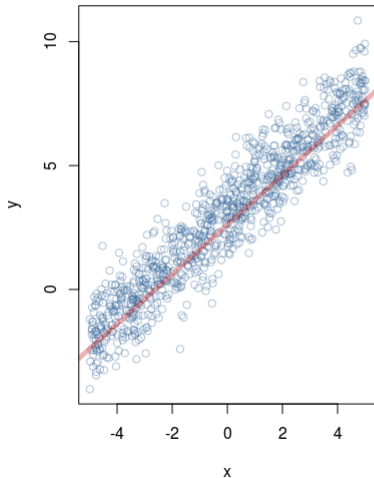


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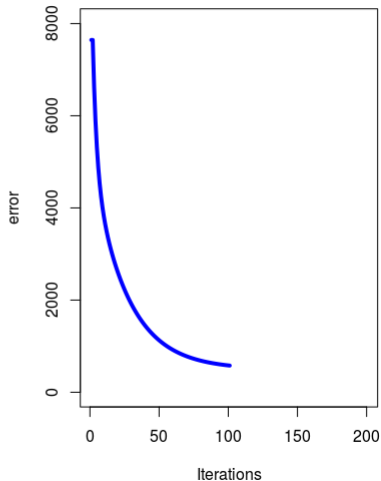


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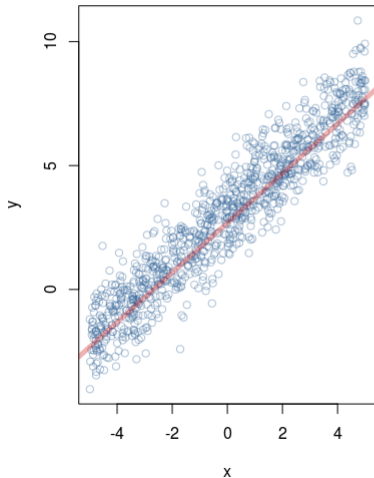


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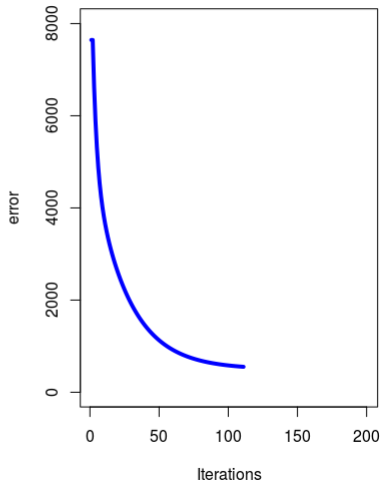


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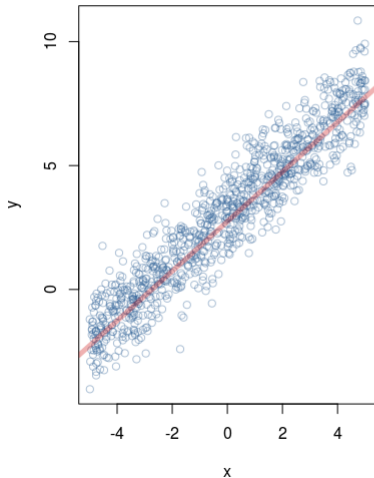


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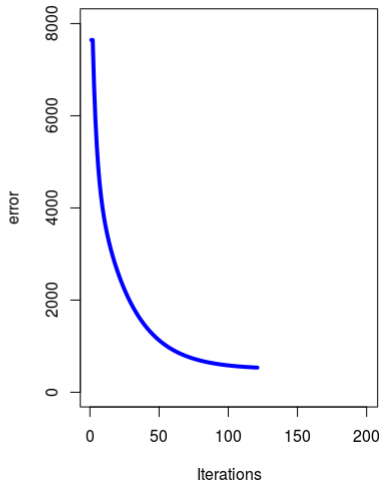


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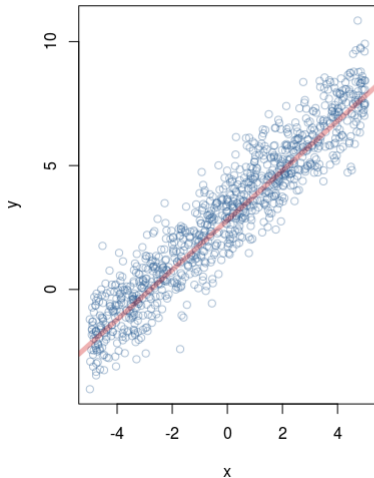


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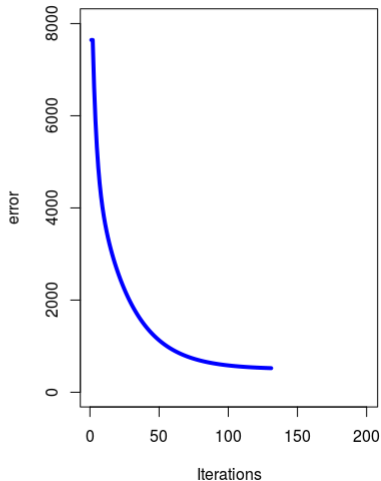


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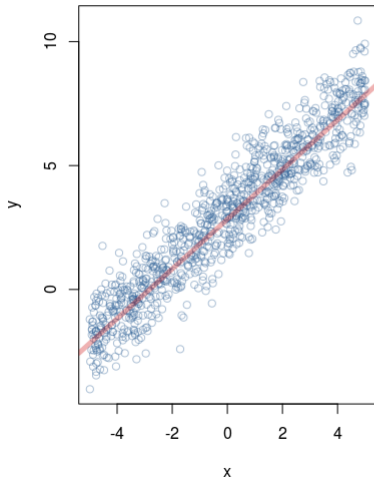
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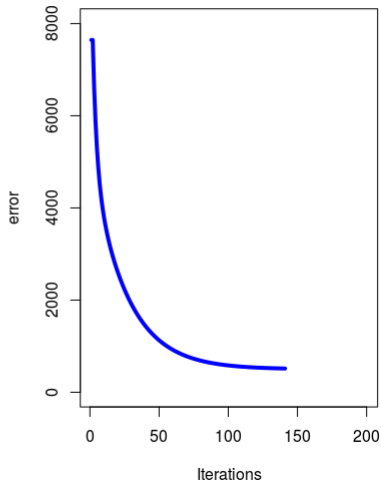


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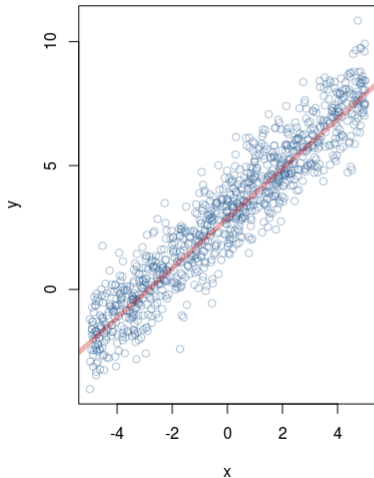


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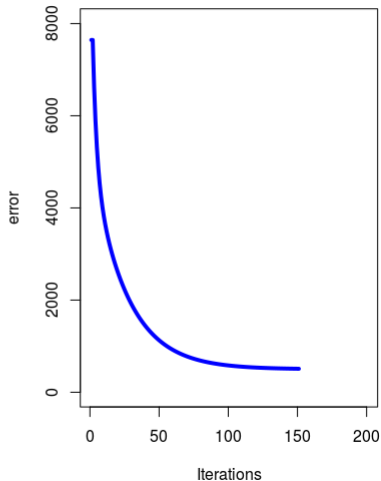


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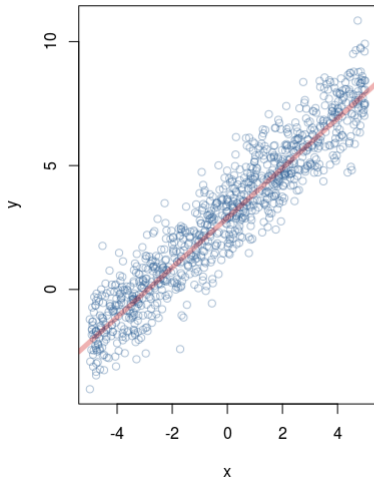


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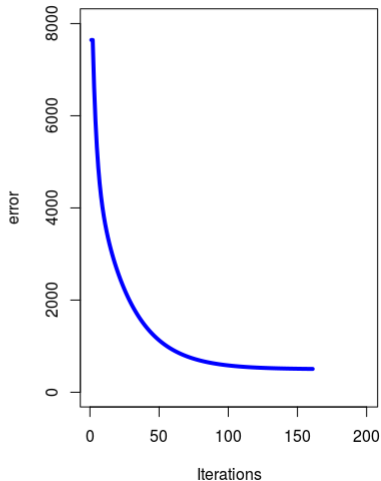


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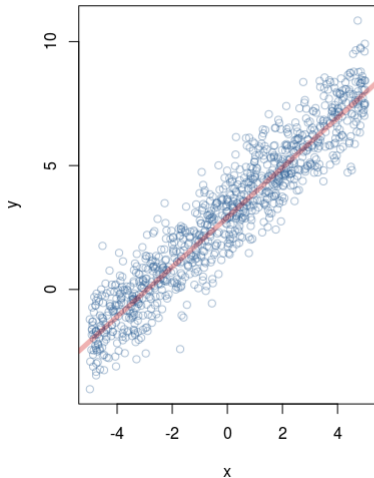


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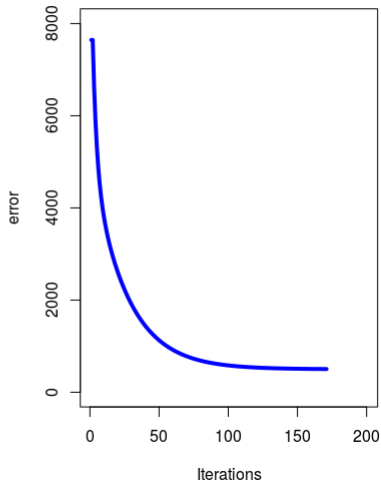


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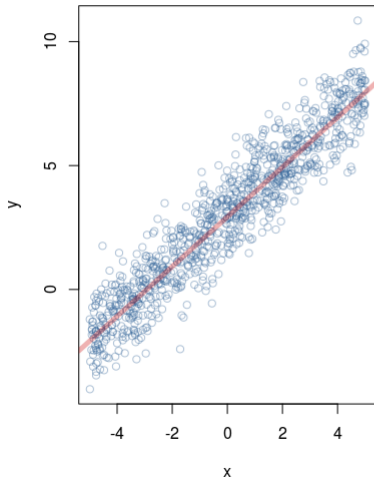


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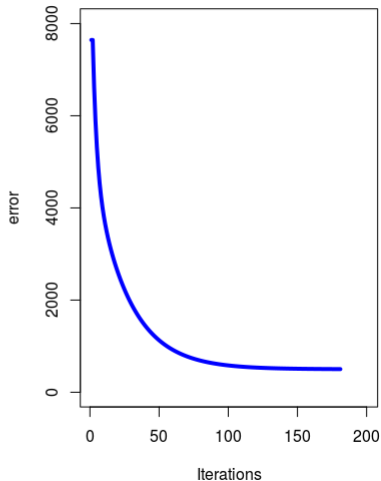


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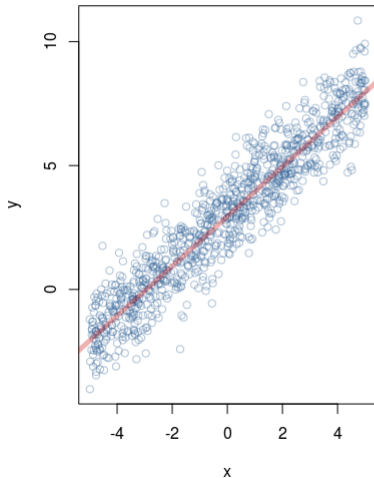


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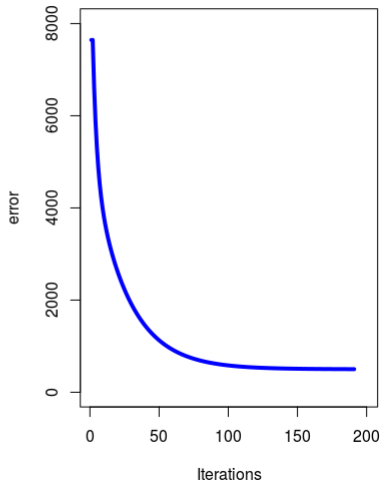


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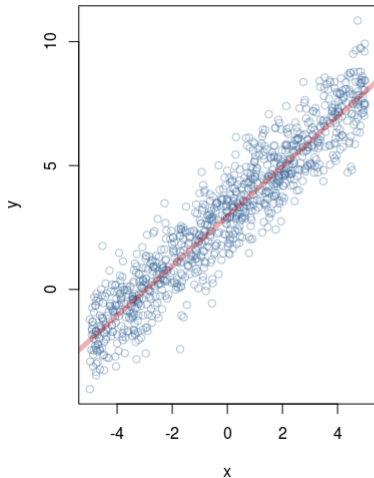


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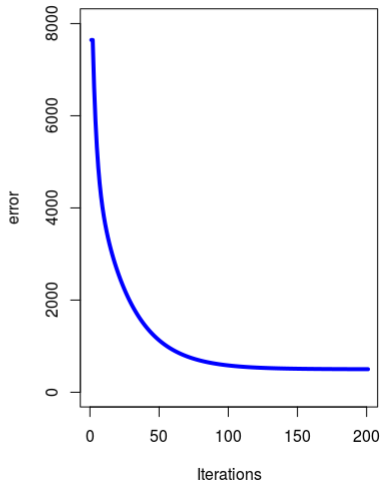


# Linear Regression - Animation

Linear regression by gradient descent



Error function



## Finding the Minimum in Dimension One

Assume  $n = 1$ . Then, the error function  $E$  is

$$E(w_0, w_1) = \frac{1}{2} \sum_{k=1}^p (w_0 + w_1 x_k - f_k)^2$$



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$$\frac{\partial E}{\partial w_0} = 0 \quad \Leftrightarrow \quad w_0 = \bar{f} - w_1 \bar{x} \quad \Leftrightarrow \quad \bar{f} = w_0 + w_1 \bar{x}$$

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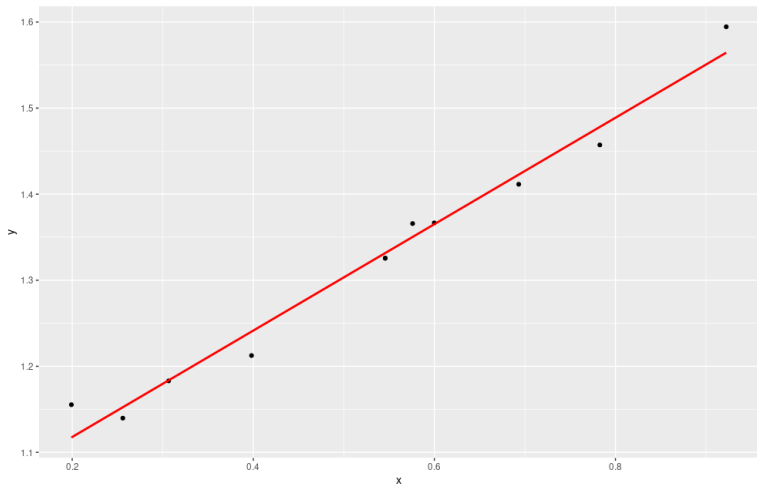
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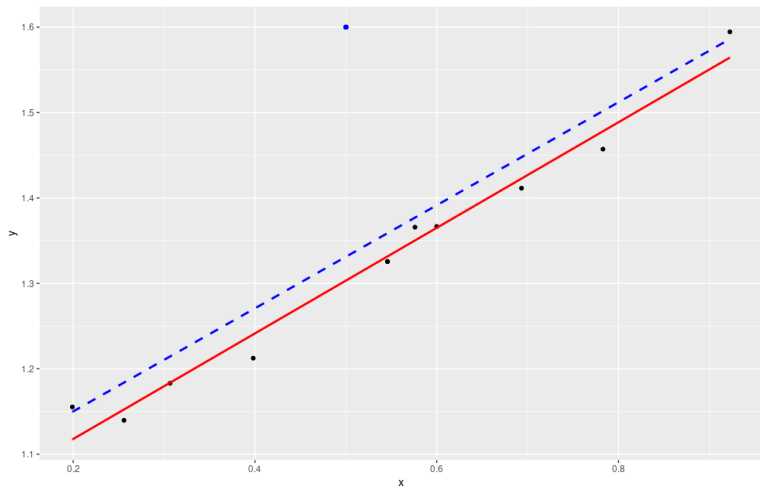
$$\frac{\partial E}{\partial w_1} = 0 \quad \Leftrightarrow \quad w_1 = \frac{\frac{1}{p} \sum_{k=1}^p (f_k - \bar{f})(x_k - \bar{x})}{\frac{1}{p} \sum_{k=1}^p (x_k - \bar{x})^2}$$

i.e.  $w_1 = \text{cov}(f, x) / \text{var}(x)$

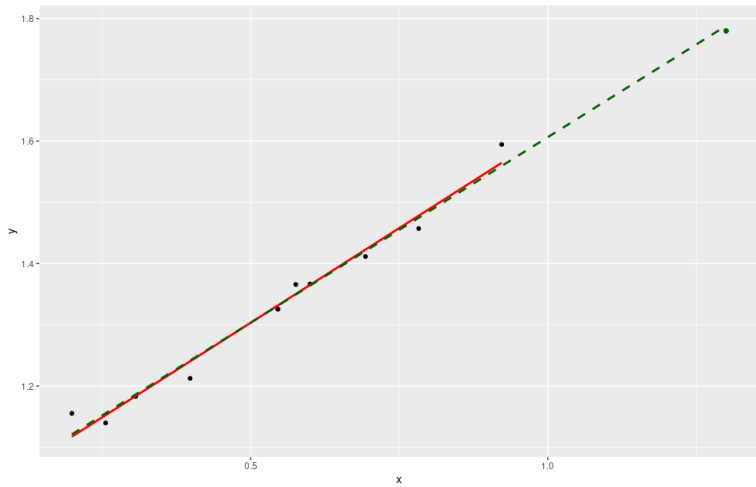
# Effect of Outliers



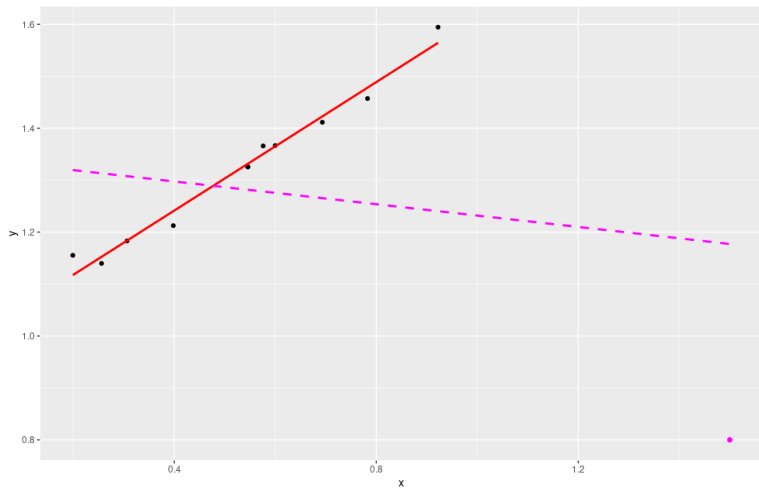
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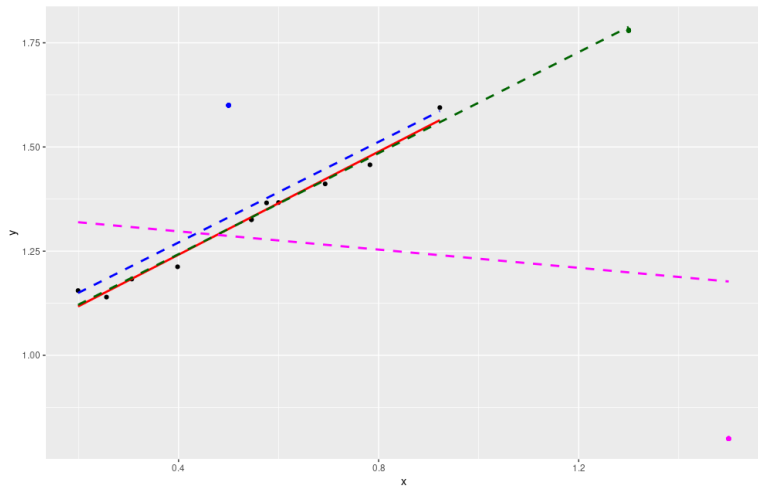
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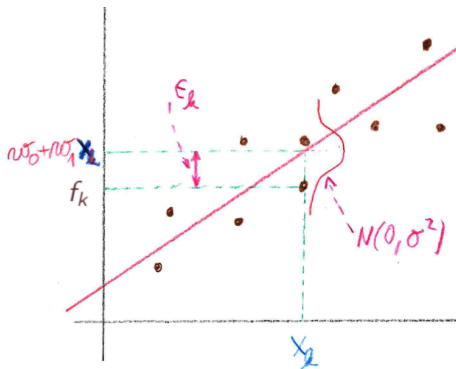
# Maximum Likelihood vs Least Squares (Dim 1)

Fix a training set  $D = \{(x_1, f_1), (x_2, f_2), \dots, (x_p, f_p)\}$

Assume that each  $f_k$  has been generated randomly by

$$f_k = (w_0 + w_1 \cdot x_k) + \epsilon_k$$

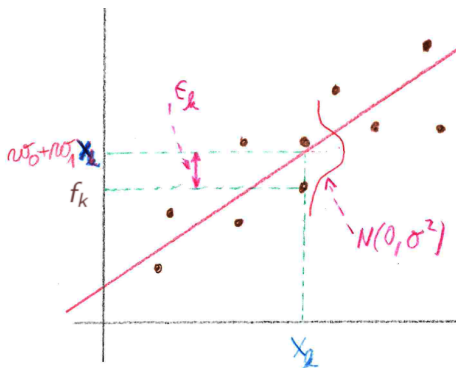
where  $w_0, w_1$  are **unknown weights**, and  $\epsilon_k$  are independent, normally distributed noise values with mean 0 and some variance  $\sigma^2$



How "probable" is it to generate the correct  $f_1, \dots, f_p$  ?



# Maximum Likelihood vs Least Squares (Dim 1)



How "probable" is it to generate the correct  $f_1, \dots, f_p$  ?

The following conditions are equivalent:

- ▶  $w_0, w_1$  minimize the squared error  $E$
- ▶  $w_0, w_1$  maximize the likelihood (i.e., the "probability") of generating the correct values  $f_1, \dots, f_p$  using  $f_k = (w_0 + w_1 \cdot x_k) + \epsilon_k$

## Comments on Linear Models

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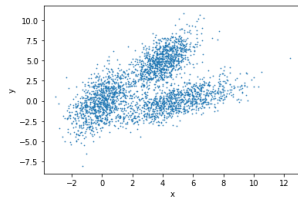
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# Unsupervised Learning

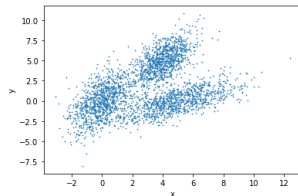
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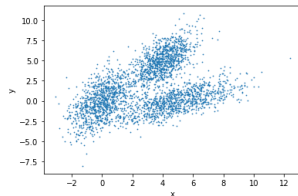


This means that the data distribution is *multimodal*, i.e., contains several regions of higher probability mass.



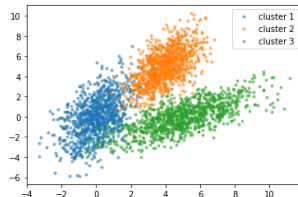
# Clustering

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We aim to group data into clusters of “similar” examples without using any additional information.  
(no supervision).

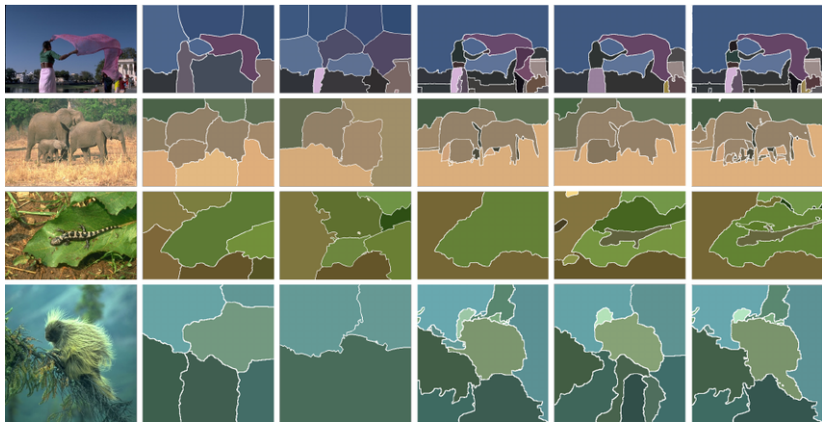


# Motivation

Clustering is useful, e.g., in

- ▶ Customer segmentation based on their purchases.
- ▶ Data exploration - identify patterns in data
- ▶ Semi-supervised learning - cluster labeled examples with the unlabeled ones
- ▶ Search engines - searching for images similar to a given image
- ▶ Image segmentation
- ▶ ...

# Segmentation



# Clustering Problem

Consider a dataset

$$D = \{\vec{x}_1, \dots, \vec{x}_p\}$$

Note that no target class/value is provided.

*Clustering* is a partition  $\mathcal{U} = \{U_1, \dots, U_K\}$  of  $D$  into  $K$  clusters.

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**For concreteness:**

- ▶ We stick with numerical features, which means that the dataset  $D = \{\vec{x}_1, \dots, \vec{x}_p\}$  contains vectors  $\vec{x}_i \in \mathbb{R}^n$ .
- ▶ Assume the Euclidean distance  $d$ .

Note that clustering may be based on completely different similarity/dissimilarity measures and non-numerical data.

# K-Means Clustering



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- ▶ An *assignment*  $q_{ij} \in \{0, 1\}$  for  $i = 1, \dots, p$  and  $j = 1, \dots, K$  of inputs  $\vec{x}_i$  to clusters  $U_j$  so that

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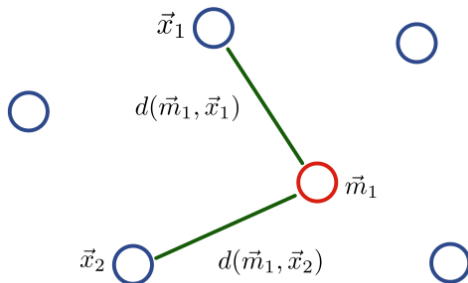
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How good is a given model?

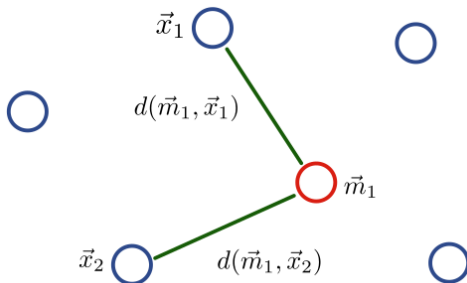
## Error Function

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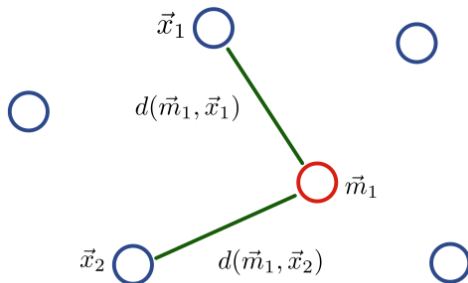
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We aim to *minimize* this error, i.e., to find proper positions of cluster prototypes and their assignment to minimize the total squared distance of examples to their prototypes.



## K-means Clustering Complexity

**The Problem** *K*-means clustering problem (optimization):

Given a set  $D = \{\vec{x}_1, \dots, \vec{x}_p\}$  where  $\vec{x}_k \in \mathbb{R}^n$  for all  $k = 1, \dots, p$  and an integer  $K$ , minimize

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**The Problem  $K$ -means clustering problem (decision):** Similar to the optimization variant except that given a constant  $c \in \mathbb{R}$  we search for  $\{q_{ij}\}, \{\vec{m}_j\}$  satisfying  $E(\{q_{ij}\}, \{\vec{m}_j\}) \leq c$ .

### Theorem

*The  $K$ -means clustering problem is NP-hard.*

For details see Aloise et al. Clustering Large Graphs via the Singular Value Decomposition, Mach Learn (2009) 75: 245–248

Complexity of clustering for many other variants has been studied, see, e.g., Cluster Analysis and Mathematical Programming by Hansen & Jaumard

# K-means Clustering Algorithm

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$$\sum_i q_{ij} d(\vec{x}_i, \vec{m}_j)^2$$

# K-means Clustering Algorithm

**The Problem:** Minimize

$$E(\{q_{ij}\}, \{\vec{m}_j\}) = \sum_{i=1}^p \sum_{j=1}^K q_{ij} d(\vec{x}_i, \vec{m}_j)^2 \text{ w.r.t. } \{q_{ij}\}, \{\vec{m}_j\}$$

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$$\sum_i q_{ij} d(\vec{x}_i, \vec{m}_j)^2$$

This is achieved by putting each prototype  $\vec{m}_j$  into the centroid of all inputs it represents:

$$\vec{m}_j = \frac{1}{\sum_{i=1}^p q_{ij}} \sum_{i=1}^p q_{ij} \vec{x}_i$$

Note that  $\sum_{i=1}^p q_{ij}$  is the size of the cluster represented by  $\vec{m}_j$ .

# K-Means Clustering Algorithm

---

**Algorithm 1** K-means clustering

---

- 1: Initialize  $K$  cluster centers  $\vec{m}_1, \vec{m}_2, \dots, \vec{m}_K$  randomly
- 2: **repeat**
- 3:     **for** each data point  $\vec{x}_i$  **do**
- 4:         Assign  $\vec{x}_i$  to the nearest centroid, i.e., set  $q_{ij} = 1$  for

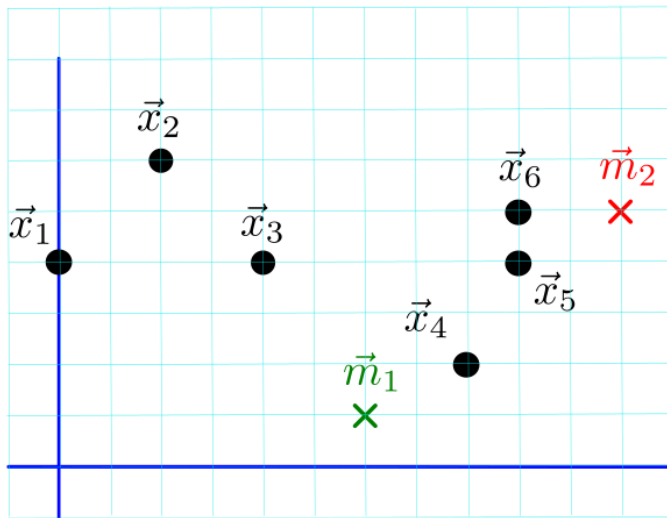
$$j = \arg \min_j d(\vec{x}_i, \vec{m}_j)^2$$

- 5:     **end for**
- 6:     **for** each cluster prototype  $\vec{m}_j$  **do**
- 7:         Update  $\vec{m}_j$  to be the centroid of all points assigned to it

$$\vec{m}_j = \frac{1}{\sum_{i=1}^p q_{ij}} \sum_{i=1}^p q_{ij} \vec{x}_i$$

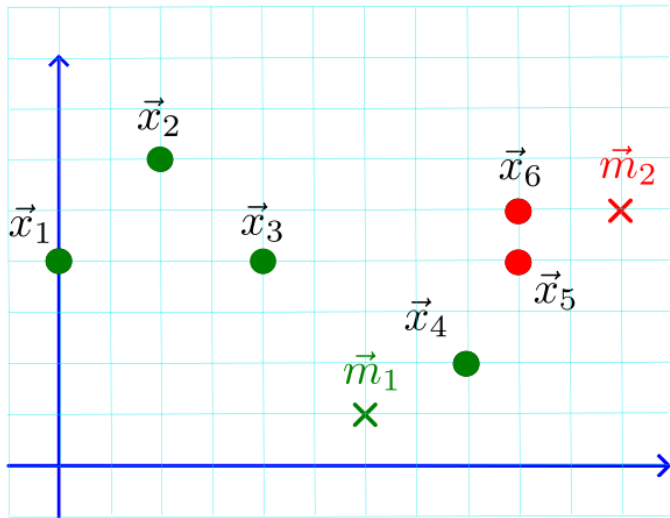
- 8:     **end for**
- 9: **until** convergence

## Example



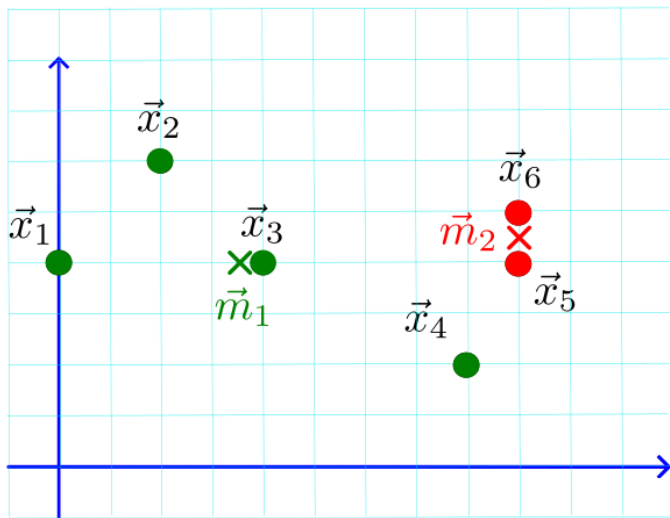


## Example



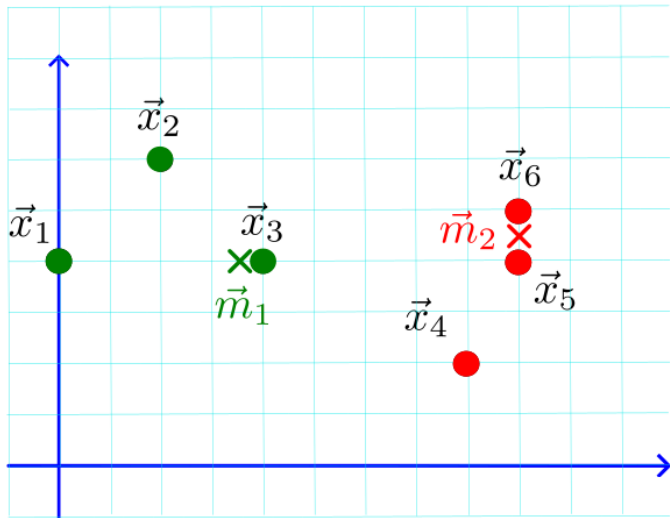
Lines 3-5: Assign examples to the prototypes.

## Example



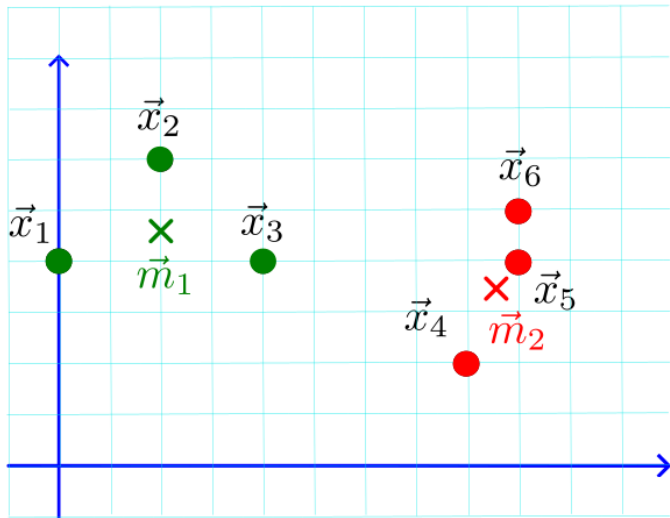
Lines 6-8: Move the prototypes to the centroids of their examples.

## Example

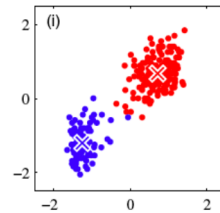
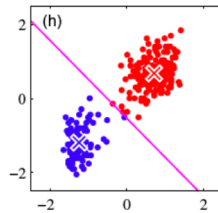
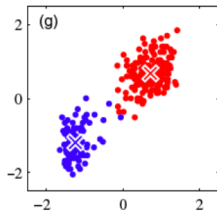
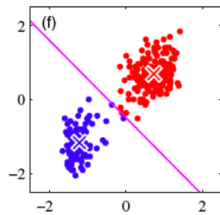
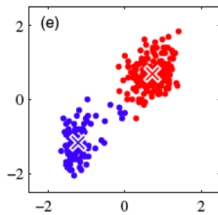
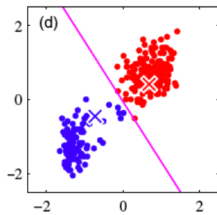
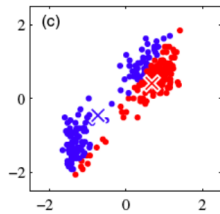
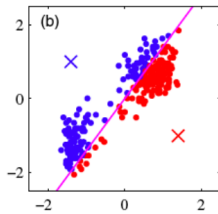
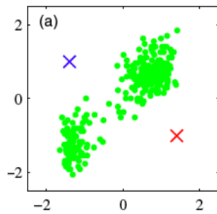


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## Example



Lines 6-8: Move the prototypes to the centroids of their examples.



## Convergence of K-means Clustering

Every step of K-means reduces the error  $E(\{q_{ij}\}, \{\vec{m}_j\})$ :

- ▶ We always assign an input vector to the closest prototype.
- ▶ We always move the prototype to be “closest” to the input vectors it represents.

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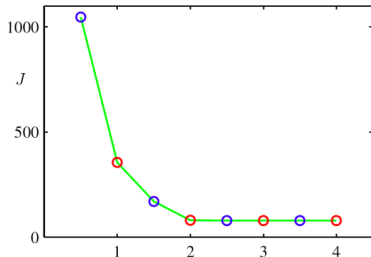
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Example error development during training. Blue circles mean reassignment, and red circles mean moving prototypes.





## Setting K - the Elbow Method

$K$ -means clustering minimizes the *inertia* measure:

$$E(\{q_{ij}\}, \{\vec{m}_j\}) = \sum_{i=1}^p \sum_{j=1}^k q_{ij} d(\vec{x}_i, \vec{m}_j)^2$$

That is the sum of squared distances of all examples of  $D$  to the cluster prototypes.

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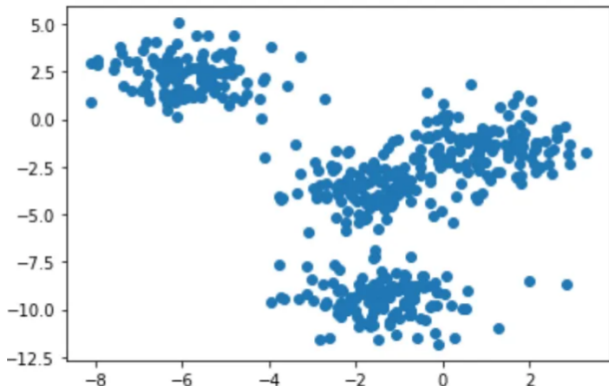
Note that the error does not consider the distance between the centers of the clusters.

Still, it is a valid measure that can be used to select the number of clusters.

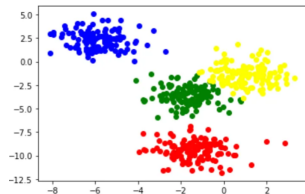
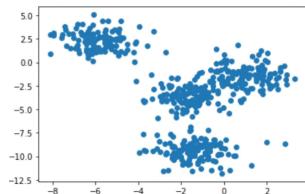
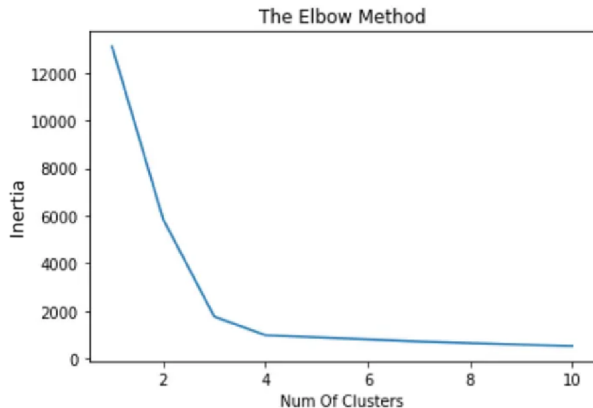
## Elbow Method

The following method for setting up the hyperparameters can be used in general. Let us illustrate the elbow method on  $K$ -means clustering with the inertia measure.

Consider the following data:



# Elbow Method



We could choose four clusters because adding more leads only to small decrements in the inertia.

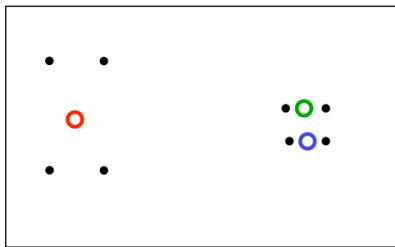
## Bad Behavior

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Some runs correspond to apparently bad solutions to the clustering problem even though a better solution exists.



Possible solution: Start the algorithm several times with random initialization of the prototypes.

# Properties of K-means Clustering

- ▶ Prototype initialization is a big issue in K-means. There are various strategies. For example:
  - ▶ Start with all centers in a single corner.
  - ▶ Include randomness in the setting of centers throughout the algorithm.
  - ▶ Initialize sequentially, always fit prototypes, and then choose a new one as far away from the others as possible.
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- ▶ Empty clusters may occur - need to resolve, e.g., by assigning the farthest point from any current prototype.

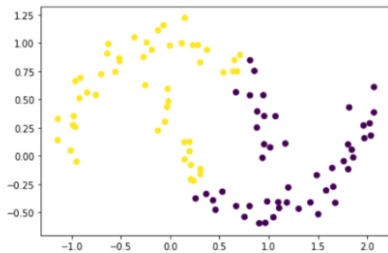
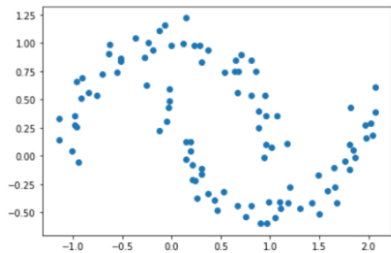
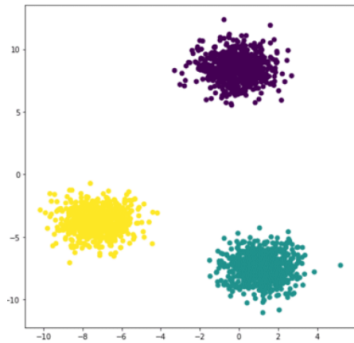
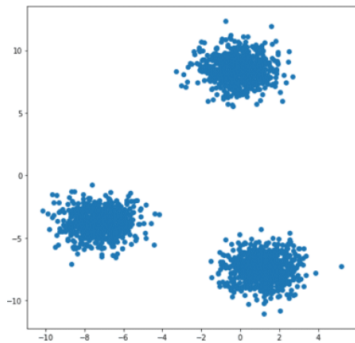


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- ▶ Other problematic properties of data include
  - ▶ non-convex clusters
  - ▶ clusters of different sizes
  - ▶ non-linearly separable clusters
  - ▶ overlapping clusters



# Agglomerative Clustering

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Consider a dataset

$$D = \{\vec{x}_1, \dots, \vec{x}_p\}$$

Here  $\vec{x}_i \in \mathbb{R}^n$  for all  $i = 1, \dots, p$ . Assume a distance  $d$  (e.g., Euclidean).

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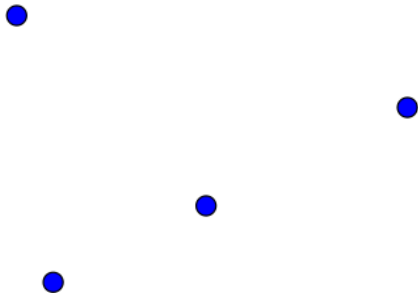
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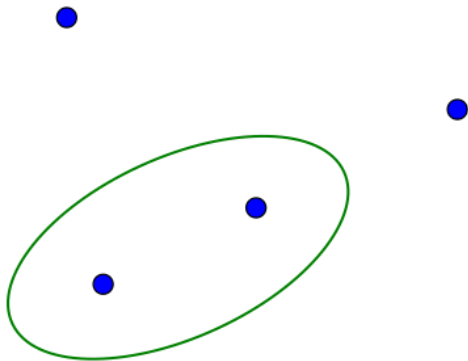
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How do we determine the closest clusters?

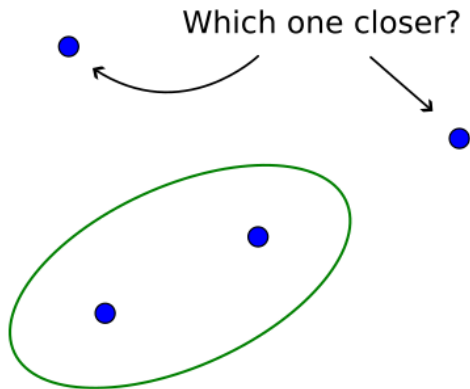
## Closest Clusters



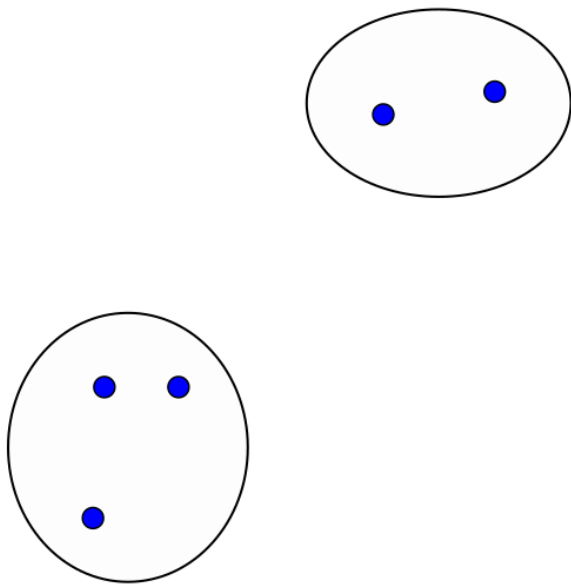
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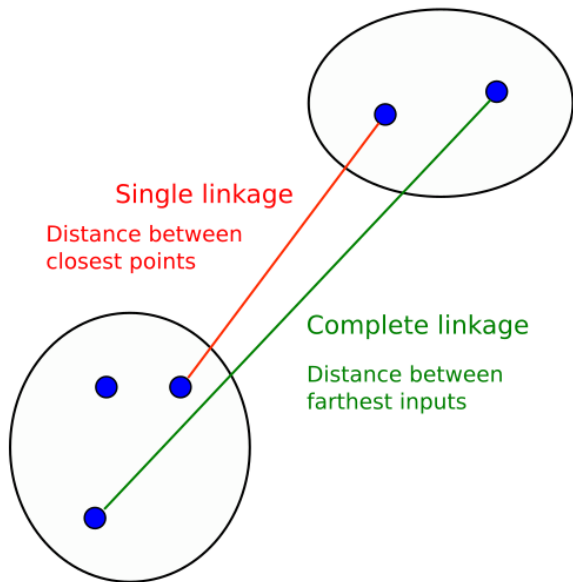
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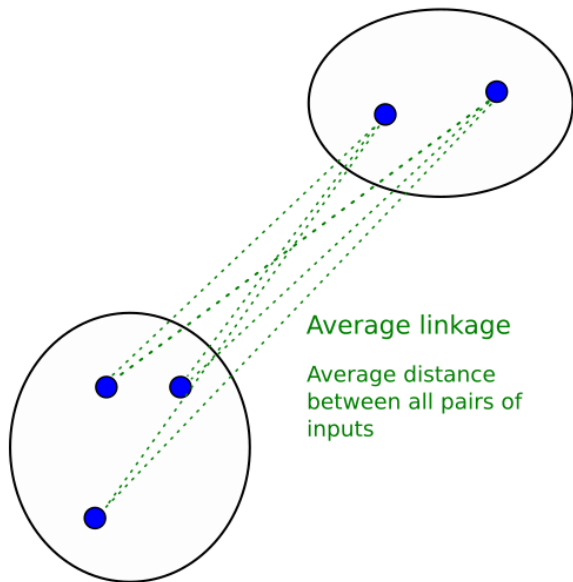
## Distance Between Clusters



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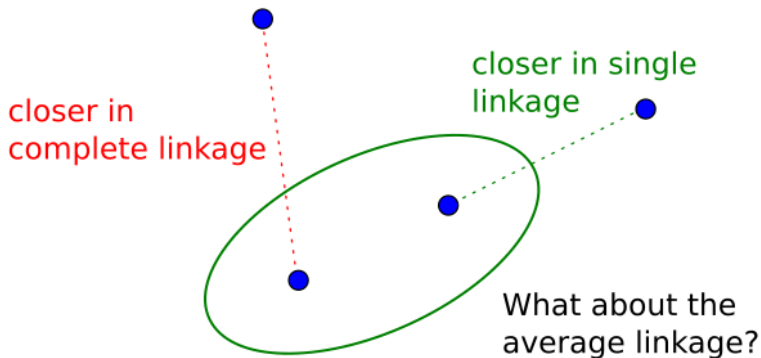


## Distance Between Clusters





## Which One is Closer?



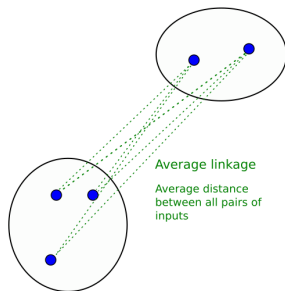
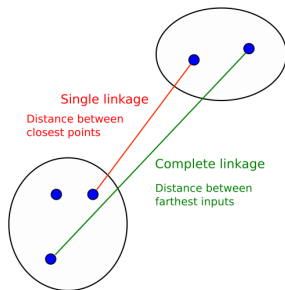
# Distance Between Clusters

Consider two clusters  $U_j, U_k \subseteq D$ .

$$\begin{aligned} \text{single\_linkage}(U_j, U_k) \\ = \min\{d(\vec{x}, \vec{z}) \mid \vec{x} \in U_j, \vec{z} \in U_k\} \end{aligned}$$

$$\begin{aligned} \text{complete\_linkage}(U_j, U_k) \\ = \max\{d(\vec{x}, \vec{z}) \mid \vec{x} \in U_j, \vec{z} \in U_k\} \end{aligned}$$

$$\begin{aligned} \text{average\_linkage}(U_j, U_k) \\ = \frac{1}{|U_j||U_k|} \sum_{\vec{x} \in U_j} \sum_{\vec{z} \in U_k} d(\vec{x}, \vec{z}) \end{aligned}$$



Each linkage can result in a different clustering.

# Agglomerative Hierarchical Clustering Algorithm

Maintain a set of clusters

Initially, each  $\vec{x}_i$  in its own cluster

**repeat**

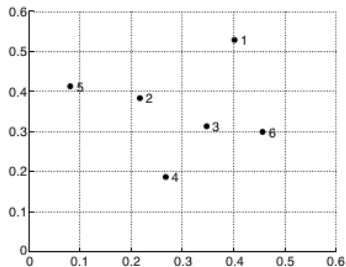
    Pick two closest clusters

        Using the distance measure  $d$  and single, average, or complete linkage.

    Merge them into a new cluster

**until** only one cluster is left

# Example

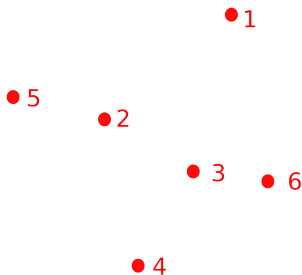


Point	<i>x</i> Coordinate	<i>y</i> Coordinate
p1	0.40	0.53
p2	0.22	0.38
p3	0.35	0.32
p4	0.26	0.19
p5	0.08	0.41
p6	0.45	0.30

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

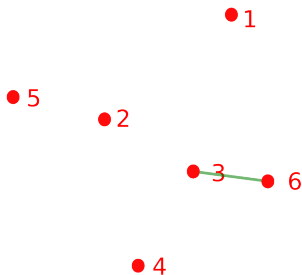
## Example - Single Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
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p5	0.34	0.14	0.28	0.29	0.00	0.39
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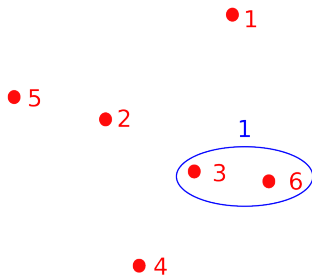


$$d(3, 6) = 0.11$$

which is the minimum  
distance between points.

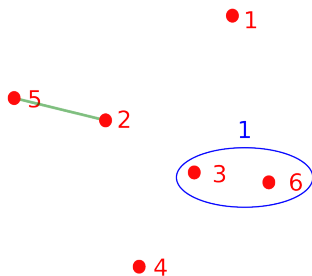
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p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
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## Example - Single Linkage

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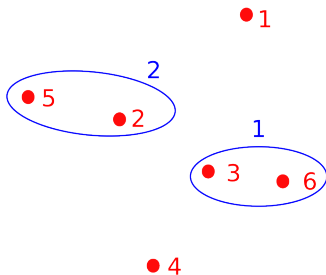
$$d(2, 5) = 0.14$$

which is the second smallest distance.



## Example - Single Linkage

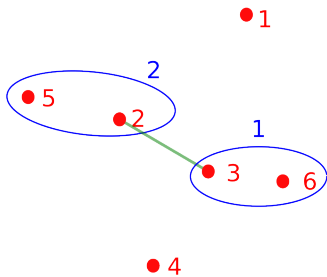
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Single Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

$$d(2, 3) = 0.15 = \min\{d(2, 3), d(2, 6), d(5, 3), d(5, 6)\}$$



which is smaller than

$$d(1, 2) = 0.24,$$

$$d(1, 3) = 0.22,$$

$$d(4, 2) = 0.2,$$

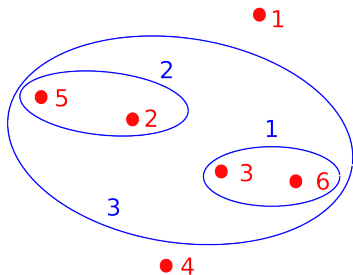
$$d(4, 3) = 0.16,$$

$$d(4, 1) = 0.37$$

the min. distances of points  
in all other pairs of clusters.

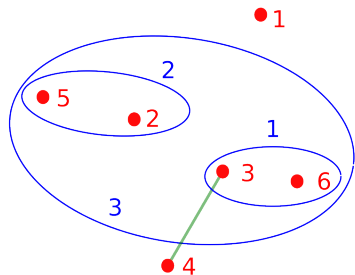
## Example - Single Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Single Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



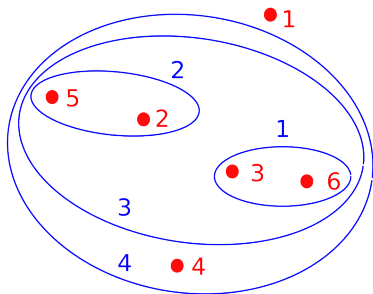
$$d(4, 3) = 0.15$$

$$= \min\{d(4, 3), d(4, 5), d(4, 2), d(4, 6)\}$$

which is smaller than  
 $d(1, 3) = 0.22$ , the distance  
of **1** to the cluster **3**.

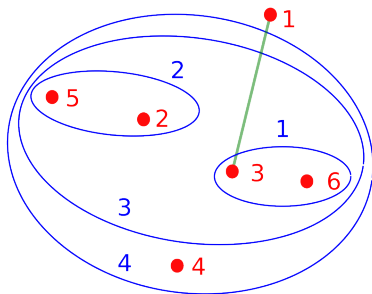
## Example - Single Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



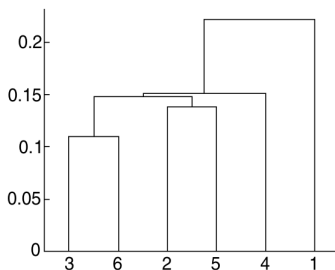
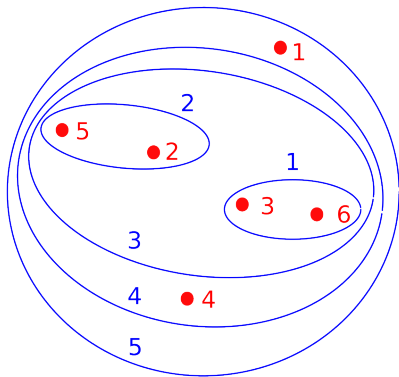
## Example - Single Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



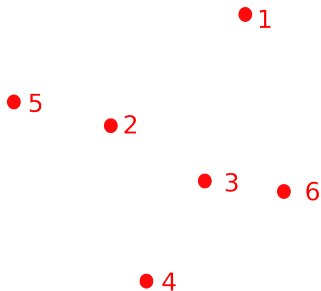
## Example - Single Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Average Linkage

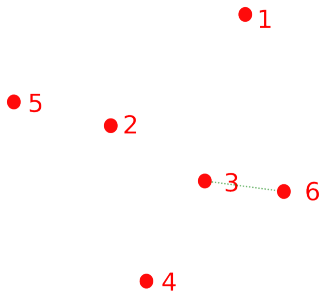
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00





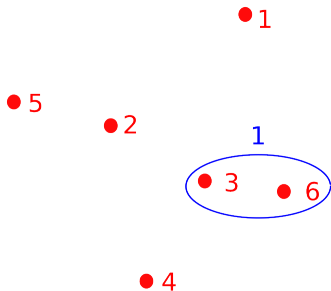
## Example - Average Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



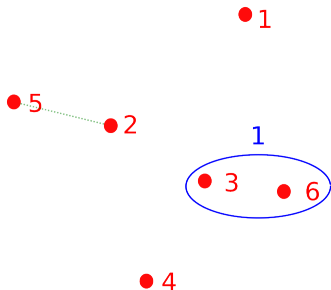
## Example - Average Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Average Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

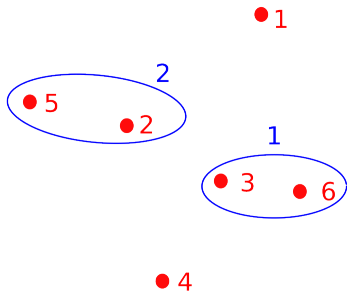


$$d(2, 5) = 0.14$$

which is second smallest distance.

## Example - Average Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Average Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

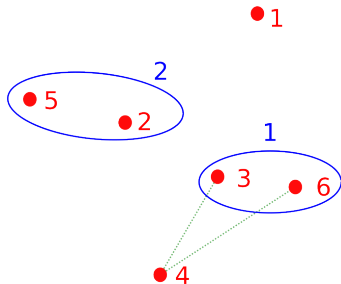
The average distance between **4** and both points of **{3,6}** is

$$\frac{1}{2}(d(4,3) + d(4,6)) = 0.19$$

which is smaller than the average distance between all points of clusters **1,2**:

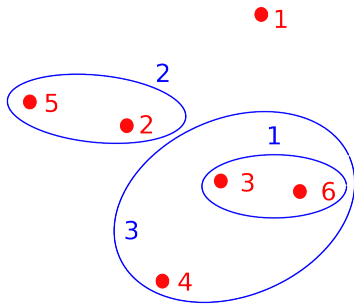
$$\frac{d(5,2) + d(5,3) + d(2,3) + d(2,6)}{4}$$

(equal to 0.205), and the average distance of **1** to any cluster.



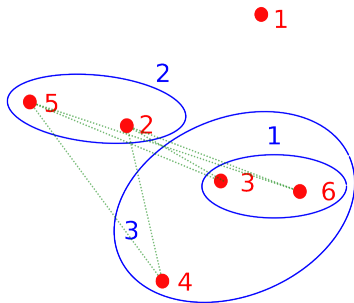
## Example - Average Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Average Linkage

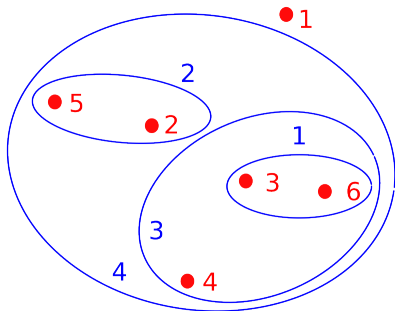
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



The average distance between clusters 2, 3 is 0.26 which is smaller than the average distance of 1 to any of the two clusters 1, 2 (the average distances are 0.273 and 0.29).

## Example - Average Linkage

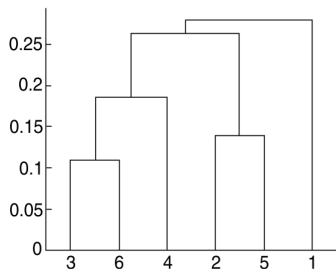
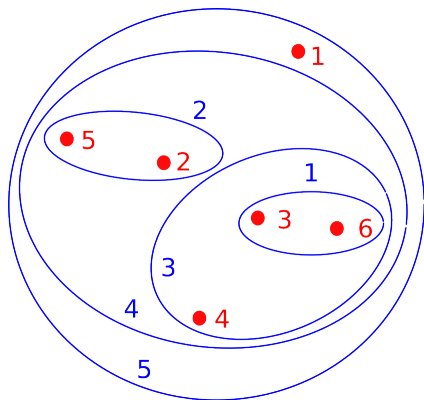
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00





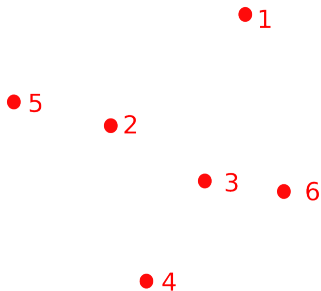
## Example - Average Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



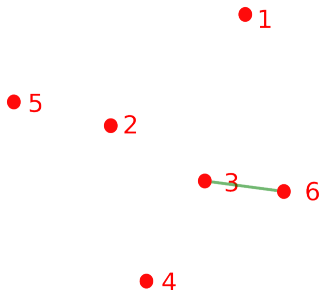
## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

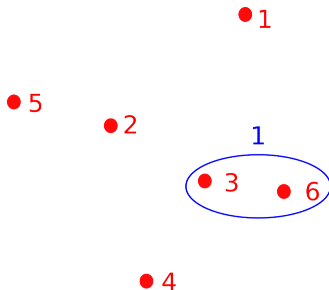


$$d(3, 6) = 0.11$$

which is the minimum  
distance between points.

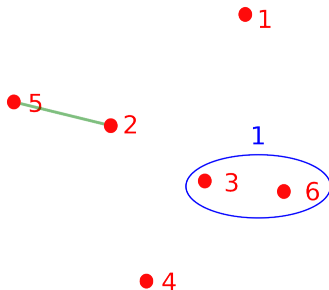
## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

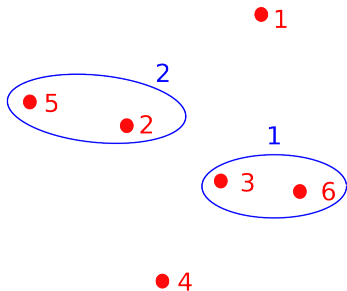


$$d(2, 5) = 0.14$$

which is the second smallest distance.

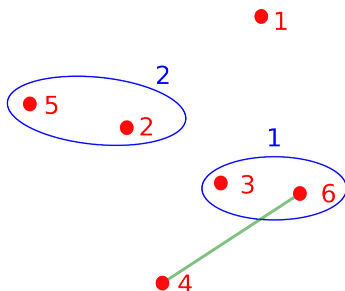
## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



$$d(4, 6) = 0.22 = \max\{d(4, 3), d(4, 6)\}$$

which is smaller than

$$d(4, 5) = 0.29,$$

$$d(1, 5) = 0.34,$$

$$d(1, 6) = 0.23,$$

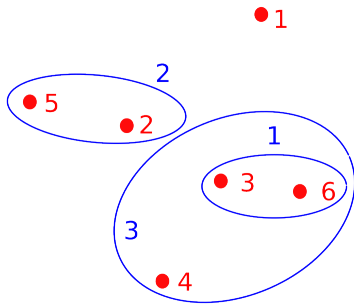
$$d(5, 6) = 0.39,$$

$$d(4, 1) = 0.37$$

the max distances of points  
in all other pairs of clusters.

## Example - Complete Linkage

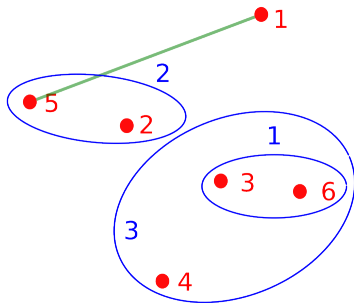
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00





## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

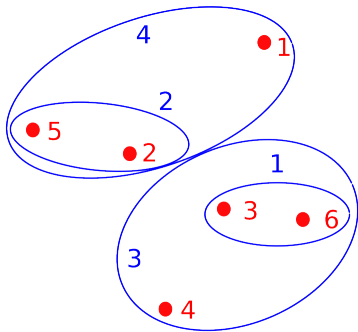


$$d(1, 5) = 0.34$$

which is smaller than  
 $d(1, 4) = 0.37$ ,  
 $d(5, 6) = 0.39$ ,  
which are the maximum  
distances of points in all  
other pairs of clusters.

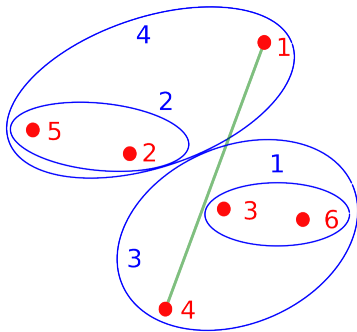
## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



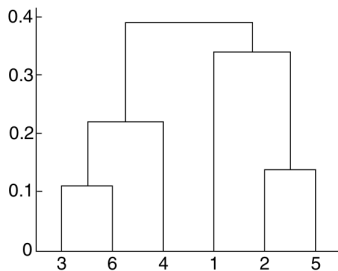
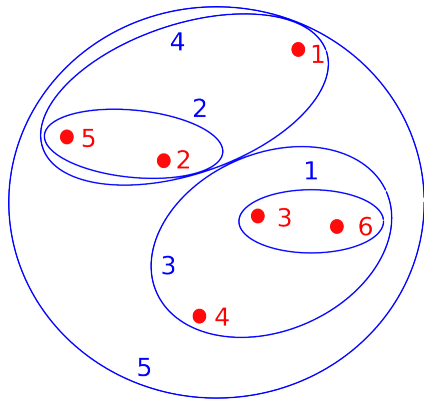
## Example - Complete Linkage

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



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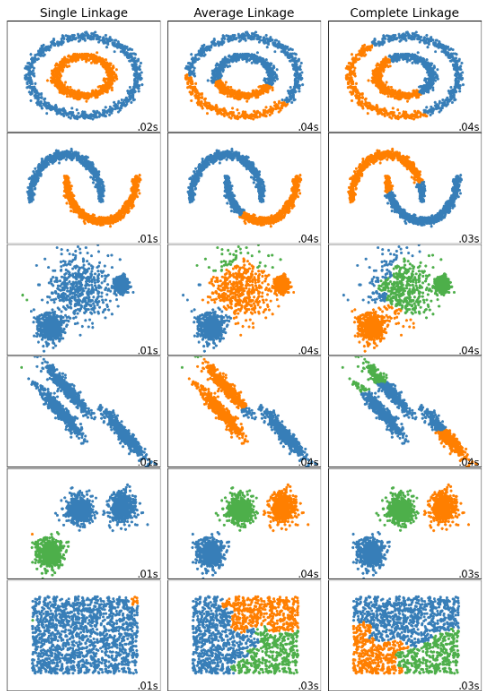


# Properties of Agglomerative Hierarchical Clustering

- ▶ Provides hierarchy of clusters - different cut levels provide different levels of coarseness of clusters
- ▶ Compared with  $k$ -means, it does not depend on the initialization and may provide better clusters than  $k$ -means.

# Properties of Agglomerative Hierarchical Clustering

- ▶ Provides hierarchy of clusters - different cut levels provide different levels of coarseness of clusters
- ▶ Compared with  $k$ -means, it does not depend on the initialization and may provide better clusters than  $k$ -means.
- ▶ Lack of global objective function
  - ▶ The agglomerative hierarchical clustering uses local criteria to decide which clusters to merge.
- ▶ Agglomerative clustering has a “rich get richer” behavior that leads to uneven cluster sizes
- ▶ Merging decision cannot be undone - bad for noisy data
- ▶ Computationally expensive.



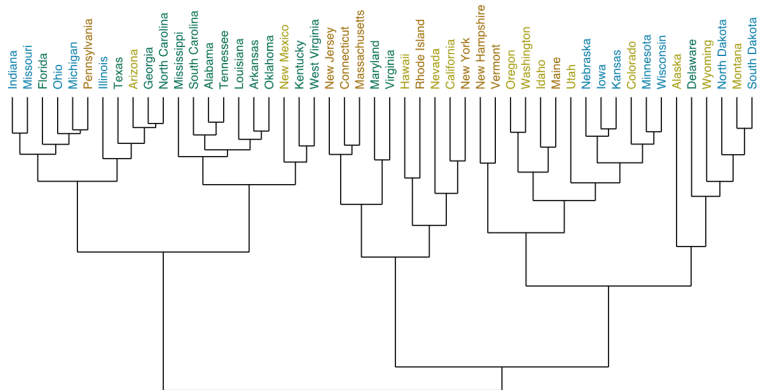
# State level statistics for US

```
# A tibble: 50 × 20
```

```
  state      homeo...1 multi...2 income med_i...3 poverty fed_s...4 smoke murder robbery
  <chr>      <dbl>    <dbl>    <dbl>    <dbl>    <dbl>    <dbl>    <dbl>    <dbl>    <dbl>
1 Alabama    71.1      15.5    22984    42081     17.1     11.7     24.8      8.2     141.
2 Alaska     64.7      24.6    30726    66521      9.5     16.8      25       4.8     80.9
3 Arizona    67.4      20.7    25680    50448     15.3      9.85    20.4      7.5    144.
4 Arkansas   67.7      15.2    21274    39267     18       9.61    23.5      6.7     91.1
5 Californ... 57.4      30.7    29188    60883     13.7      8.89    15.2      6.9    176.
6 Colorado   67.6      25.6    30151    56456     12.2      9.15    19.9      3.7     84.6
7 Connecti... 69.2      34.6    36775    67740      9.2     14.8     16.5      2.9    113
8 Delaware   73.6      17.7    29007    57599     11       8.89    20.7      4.4    155.
9 Florida    69.7       30     26551    47661     13.8      9.62    21.6       5     169.
10 Georgia    67.2      20.5    25134    49347     15.7      8.88    22.2      6.2    155.
# ... with 40 more rows, 10 more variables: agg_assault <dbl>, larceny <dbl>,
#   motor_theft <dbl>, soc_sec <dbl>, nuclear <dbl>, coal <dbl>,
#   tr_deaths <dbl>, tr_deaths_no_alc <dbl>, unempl <dbl>, popdens2010 <dbl>,
#   and abbreviated variable names 1homeownership, 2multiunit, 3med_income,
#   4fed_spend
```

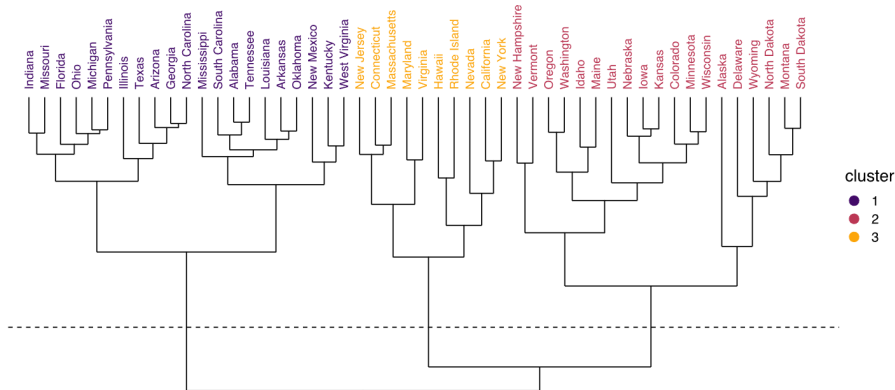


# State level statistics for US

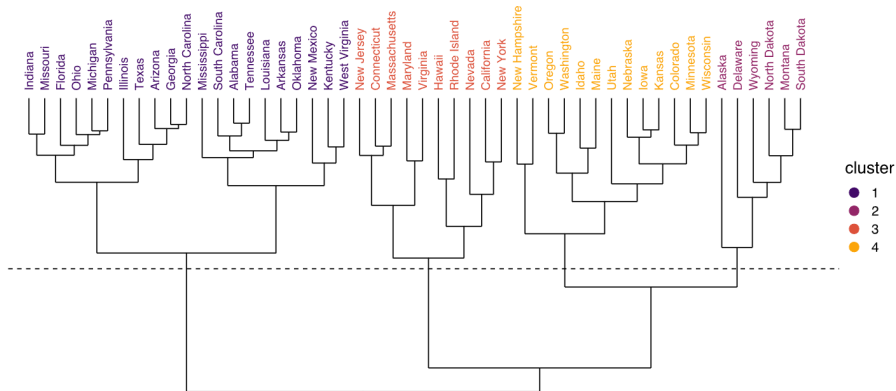


- Midwest
- Northeast
- South
- West

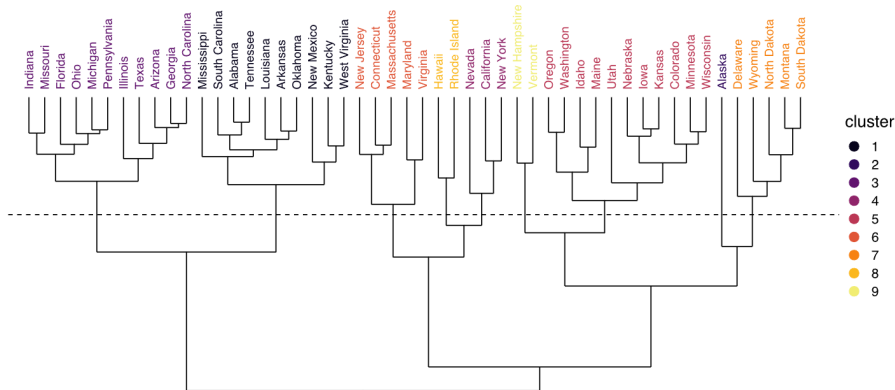
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# Cluster Validation

# Cluster Validity

For supervised classification (= we have class labels) we have a variety of measures to evaluate how good our model is:  
Accuracy, Precision, Recall,  $F_1$ , etc.

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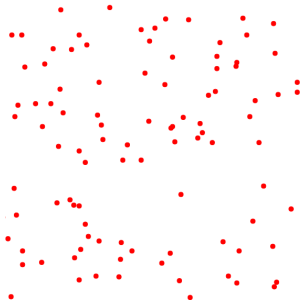
For supervised classification (= we have class labels) we have a variety of measures to evaluate how good our model is:  
Accuracy, Precision, Recall,  $F_1$ , etc.

For cluster analysis (=unsupervised learning), the analogous question is:

How to evaluate the “goodness” of the resulting clusters?

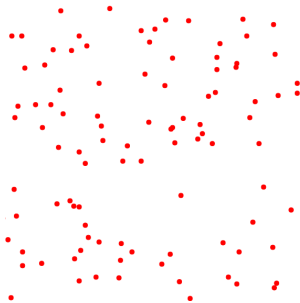
Keep in mind that the dataset can be large and high-dimensional.  
Visualization might be difficult.

Random points:

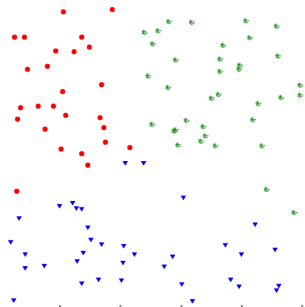




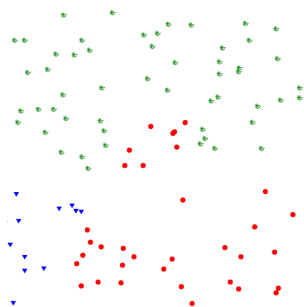
Random points:



K-means



Hierarchical



# Different Aspects of Cluster Validation

1. Determining the **clustering tendency** of a set of data, i.e., distinguishing whether non-random structure exists in the data (e.g., to avoid overfitting).

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4. **Compare clusterings** to determine which is better.
5. Determining the '**correct**' number of clusters.

For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.

# Measures of Cluster Validity

Numerical measures applied to judge various aspects of cluster validity are classified into the following three types.

- ▶ **Internal Index:** Used to measure the goodness of a clustering structure without respect to external information.
- ▶ **External Index:** Used to measure the extent to which cluster labels match externally supplied class labels.
- ▶ **Relative Index:** Used to compare two different clusterings or clusters.

## Internal Index

Consider a dataset

$$D = \{\vec{x}_1, \dots, \vec{x}_p\}$$

Assume that a clustering algorithm produced a partition  $\mathcal{U} = \{U_1, \dots, U_K\}$  of  $D$  into  $K$  clusters.

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We aim to measure the clustering's “niceness” (??)

Assume that we have a distance measure  $d$  measuring how far apart the objects being clustered.

**For concreteness:**

- ▶ We stick with numerical features, which means that the dataset  $D = \{\vec{x}_1, \dots, \vec{x}_p\}$  contains vectors  $\vec{x}_i \in \mathbb{R}^n$ .
- ▶ Assume the Euclidean distance  $d$ .

Note that the validity measures may be based on completely different similarity/dissimilarity measures and non-numerical data.

## Cohesion and Separation

Consider a dataset  $D = \{\vec{x}_1, \dots, \vec{x}_p\}$  and its clustering  $\mathcal{U} = \{U_1, \dots, U_K\}$ .

Let us utilize the concept of distance to cluster prototypes and consider the distance between prototypes.

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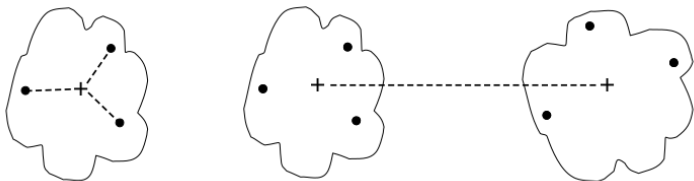
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- ▶ any other notion of dissimilarity based on the application.

We consider the notions of *cohesion* (proximity of examples within clusters) and *separation* (proximity of clusters).

# Prototype-based Cohesion and Separation



**Prototype-based cohesion** = the similarity of examples within a given cluster to a prototype of the cluster (e.g., centroid).

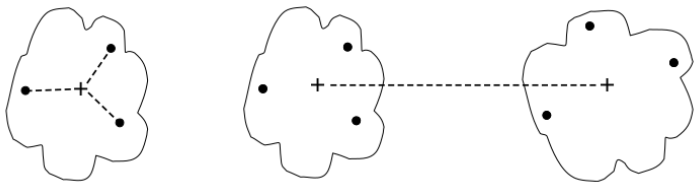
Given a cluster  $U_j \in \mathcal{U}$  and its prototype  $\vec{m}_j \in \mathbb{R}^n$ ,

$$cohesion(U_j) = \sum_{\vec{x} \in U_j} proximity(\vec{x}, \vec{m}_j)$$

Note that the prototype **does not** have to be an element of  $U_j$ .

Intuitively, cohesion is the proximity of cluster's examples and a point somewhere "between" all examples of the cluster.

# Prototype-based Cohesion and Separation



**Prototype-based separation** = dissimilarity of prototypes of different clusters.

Given a cluster  $U_j \in \mathcal{U}$ , its prototype  $\vec{m}_j \in \mathbb{R}^n$ , and a prototype of all examples  $\vec{m} \in \mathbb{R}^n$  (e.g. the centroid of all examples)

$$separation(U_j) = proximity(\vec{m}_j, \vec{m})$$

Intuitively, separation is the proximity of the cluster's examples to the dataset's center.

## Prototype-based Cohesion and Separation

Summarize the prototype-based cohesion and separation as follows:

$$\begin{aligned} \text{cohesion}(\mathcal{U}) &= \sum_{j=1}^K \text{cohesion}(U_j) \\ &= \sum_{j=1}^K \sum_{\vec{x} \in U_j} \text{proximity}(\vec{x}, \vec{m}_j) \end{aligned}$$



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There is an interesting relationship between the above measures and the squared distances to the prototype of the whole dataset  $\vec{m}$ .

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Consider a dataset  $D = \{\vec{x}_1, \dots, \vec{x}_p\}$  and its clustering  $\mathcal{U} = \{U_1, \dots, U_K\}$  of  $D$ .

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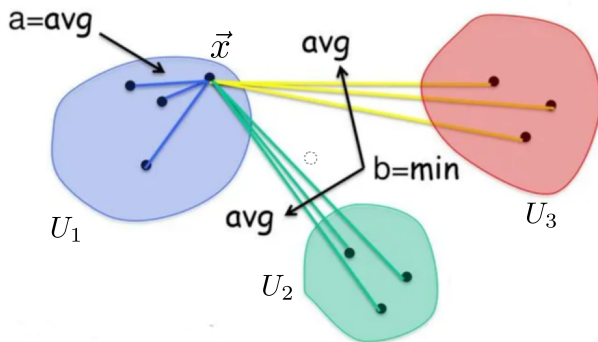
The following holds:

$$\text{TSS} = cohesion(\mathcal{U}) + separation(\mathcal{U})$$

Note that TSS is determined by  $D$ .

# Silhouette Score

*Silhouette score* can be used to measure both qualities of clustering from the point of view of individual examples and from the point of view of the overall clustering.



$$\text{silhouette}(\vec{x}) = \frac{b - a}{\max\{a, b\}}$$

## Silhouette Score

Consider a clustering  $\mathcal{U} = \{U_1, \dots, U_k\}$  and  $\vec{x} \in U_j$ .



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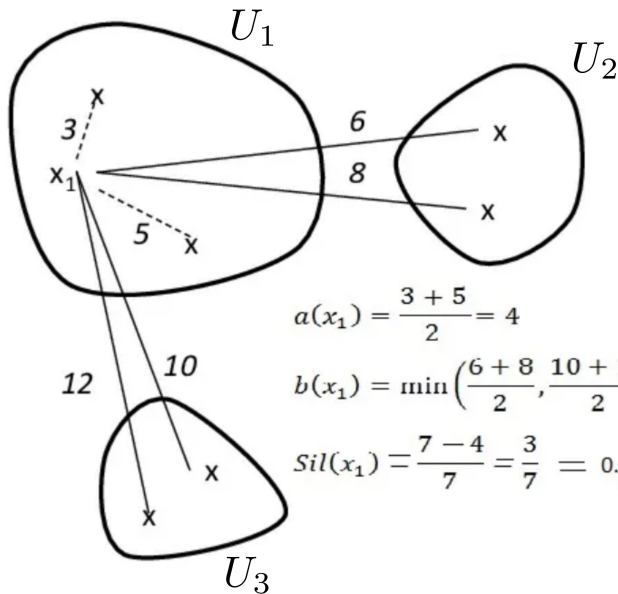
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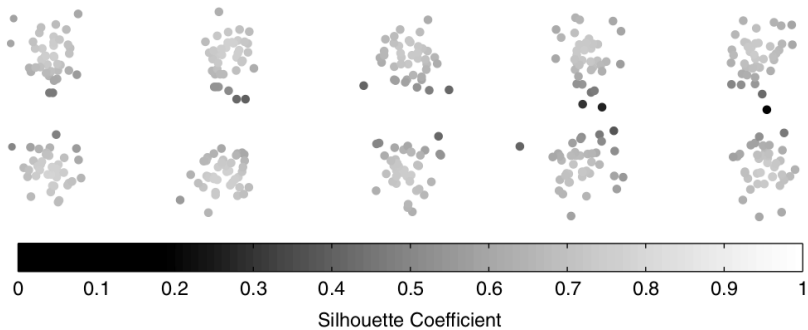
$$\textit{silhouette}(\vec{x}) = \frac{b(\vec{x}) - a(\vec{x})}{\max\{a(\vec{x}), b(\vec{x})\}}$$

Else, we define  $\textit{silhouette}(\vec{x}) = 0$ .

## Example



## Example



# Silhouette for Clusters and Clusterings

We have defined the silhouette for a single  $\vec{x} \in D$ .

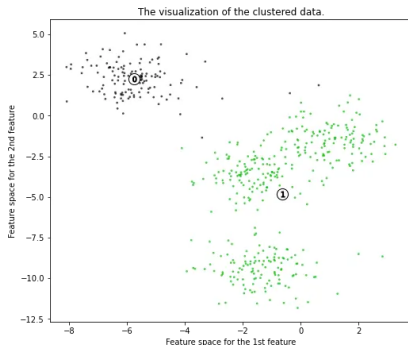
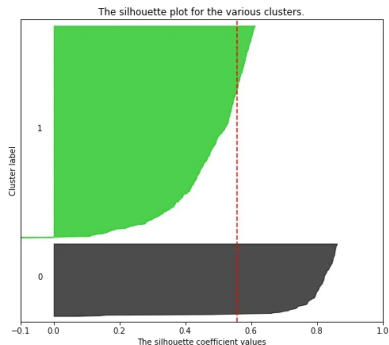
To obtain the silhouette score for a whole cluster  $U_j$  or for  $D$  we summarize using simple averaging:

$$\text{silhouette}(U_j) = \frac{1}{|U_j|} \sum_{\vec{x} \in U_j} \text{silhouette}(\vec{x})$$

$$\text{silhouette}(D) = \frac{1}{|D|} \sum_{\vec{x} \in D} \text{silhouette}(\vec{x})$$

# Example

**Silhouette analysis for KMeans clustering on sample data with  $n\_clusters = 2$**

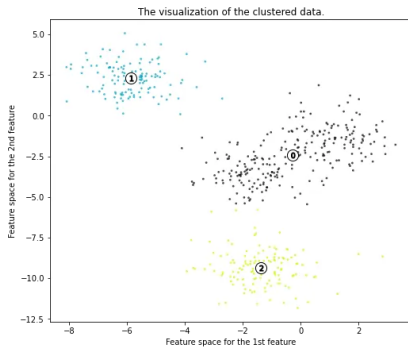
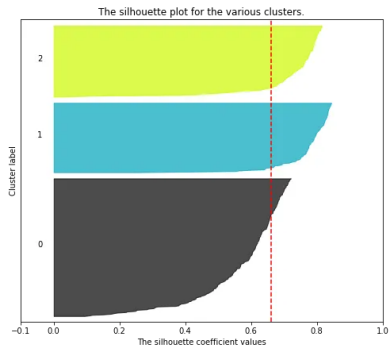


The colored graphs on the left are silhouette scores of the individual elements of clusters.

The red vertical line denotes the silhouette score for the whole dataset.

# Example

**Silhouette analysis for KMeans clustering on sample data with  $n\_clusters = 3$**



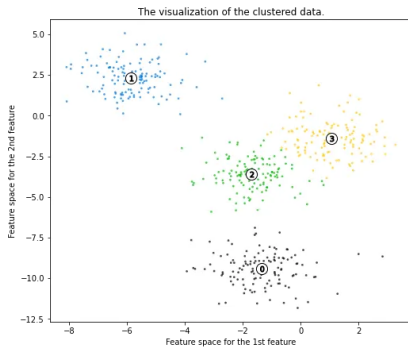
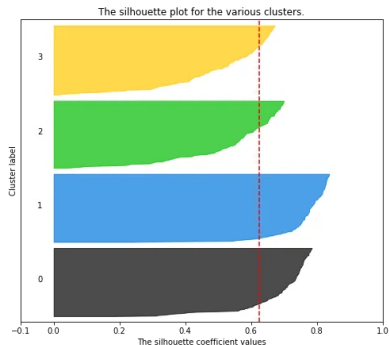
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The red vertical line denotes the silhouette score for the whole dataset.



# Example

**Silhouette analysis for KMeans clustering on sample data with  $n\_clusters = 4$**

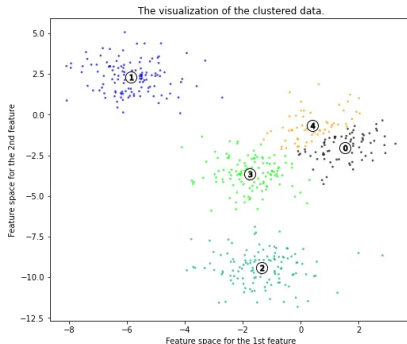
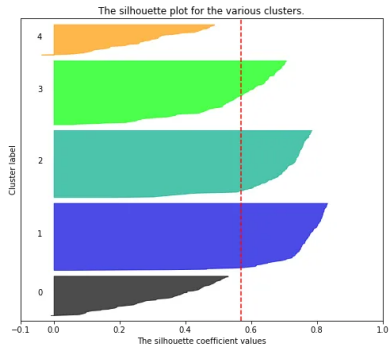


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# Example

**Silhouette analysis for KMeans clustering on sample data with  $n\_clusters = 5$**

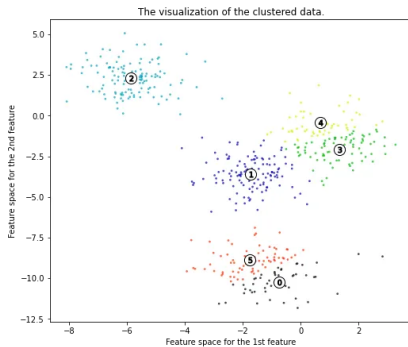
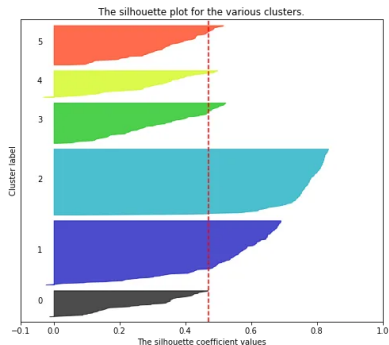


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# Example

**Silhouette analysis for KMeans clustering on sample data with  $n\_clusters = 6$**



The colored graphs on the left are silhouette scores of the individual elements of clusters.

The red vertical line denotes the silhouette score for the whole dataset.

Consider a *supervised learning* dataset

$$D = \{(\vec{x}_1, c_1), \dots, (\vec{x}_p, c_p)\}$$

Here  $c_i \in C$  is a class of  $\vec{x}_i$ .

Assume that a clustering algorithm produced a partition  $\mathcal{U} = \{U_1, \dots, U_K\}$  of  $D$  into  $K$  clusters.

We measure how the clustering conforms with the given classes.

# Purity

Consider the clustering to be a classification model.

Define a classifier  $h : D \rightarrow C$  such that given  $\vec{x}_i \in U_j \in \mathcal{U}$

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Is it a good measure?

Probably not; many clusters lead to high purity (each element in its own cluster means purity = 1).

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- ▶ TP = number of examples of the same class and the same cluster

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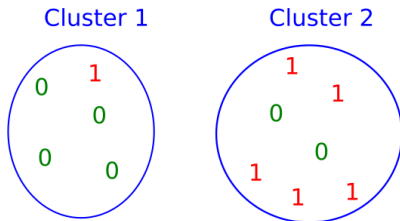
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Now, we may apply all the measures from the supervised model.

# Example



$$\begin{aligned} TP &= \binom{4}{2} + \binom{5}{2} + \binom{2}{2} \\ &= 6 + 10 + 1 = 17 \end{aligned}$$

$$TN = 4 * 5 + 1 * 2 = 22$$

$$FP = 1 * 4 + 5 * 2 = 14$$

$$FN = 1 * 5 + 4 * 2 = 13$$

		Cluster	
		<i>same</i>	<i>diff</i>
Class	<i>same</i>	TP=17	FN=13
	<i>diff</i>	FP=14	TN=22

## Rand Index

Accuracy (in this area known as *Rand index*) is

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Note that the Rand index can be used to compare two clusterings: Simply consider class labels to be indicators of clusters.

Similarly, we may compute the other measures such as Precision, Recall, and  $F_1$  with all their benefits and limitations.

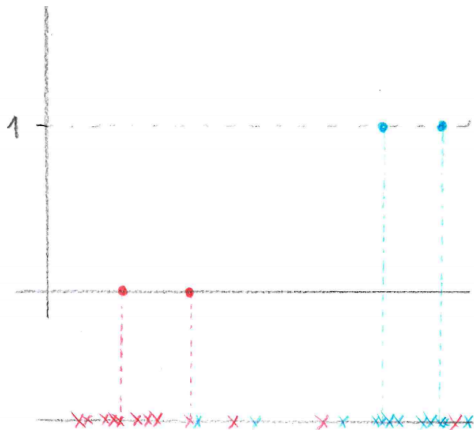


# Logistic Regression

# What about classification using regression?

Binary classification: Desired outputs 0 and 1

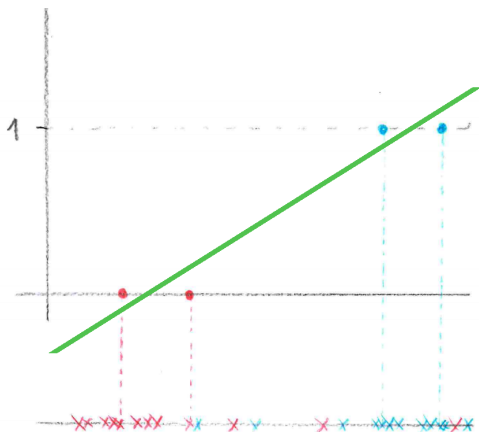
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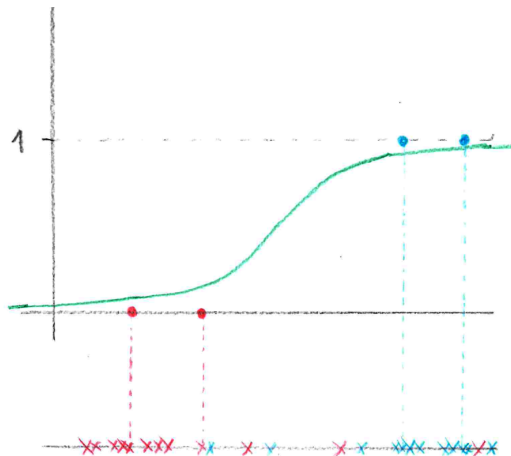


... does not capture the probability well (it is not probability at all)

# What about classification using regression?

Binary classification: Desired outputs 0 and 1

... we want to capture the probability distribution of the classes



... logistic sigmoid  $\frac{1}{1+e^{-(\vec{w} \cdot \vec{x})}}$  is much better!

# Logistic Regression

**Logistic regression** model  $h[\vec{w}]$  is determined by a vector of weights  $\vec{w} = (w_0, w_1, \dots, w_n) \in \mathbb{R}^{n+1}$  as follows:

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Given  $\vec{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$ ,

$$h[\vec{w}](\vec{x}) := \frac{1}{1 + e^{-(w_0 + \sum_{k=1}^n w_k x_k)}} = \frac{1}{1 + e^{-\vec{w} \cdot \tilde{\mathbf{x}}}}$$

Here

$$\tilde{\mathbf{x}} = (x_0, x_1, \dots, x_n) \quad \text{where } x_0 = 1$$

is the *augmented feature vector*.

## But what is the meaning of the sigmoid?

The model gives probability  $h[\vec{w}](\vec{x})$  of the class 1 given an input  $\vec{x}$ .  
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Denote by  $\bar{h}$  the probability  $P(Y = 1 \mid X = \vec{x})$ , i.e., the “true” probability of the class 1 given features  $\vec{x}$ .

---

The probability  $\bar{h}$  cannot be easily modeled using a linear function (the probabilities are between 0 and 1).



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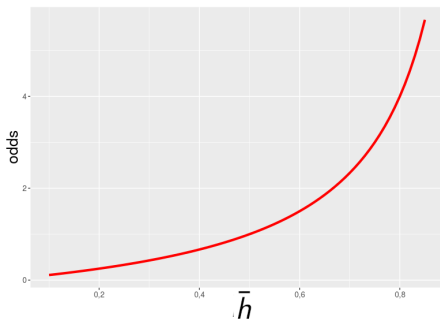
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What about **odds** of the class 1?

$$\text{odds}(\bar{h}) = \frac{\bar{h}}{1 - \bar{h}}$$



Better, at least it is unbounded on one side ...

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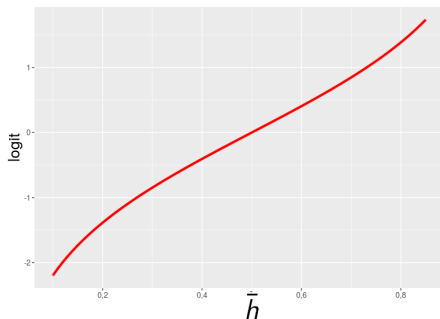
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What about **log odds (aka logit)** of the class 1?

$$\begin{aligned} \text{logit}(\bar{h}) &= \\ &\log(\bar{h}/(1 - \bar{h})) \end{aligned}$$



Looks almost linear, at least for probabilities not too close to 0 or 1 ...

## But what is the meaning of the sigmoid?

Assume that  $\bar{h}$  is the actual probability of the class 1 for an “object” with features  $\vec{x} \in \mathbb{R}^n$ . Put

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$$\bar{h} = \frac{1}{1 + e^{-\vec{w} \cdot \vec{x}}} = h[\vec{w}](\vec{x})$$

If we model log odds using a linear function, the probability is obtained by applying the logistic sigmoid on the result of the linear function.

# Logistic Regression

- ▶ Given a set  $D$  of training samples:

$$D = \{(\vec{x}_1, c_1), (\vec{x}_2, c_2), \dots, (\vec{x}_p, c_p)\}$$

Here  $\vec{x}_k = (x_{k1} \dots, x_{kn}) \in \mathbb{R}^n$  and  $c_k \in \{0, 1\}$ .

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- ▶ **Binary Cross-entropy:**

$$E(\vec{w}) = - \sum_{k=1}^p c_k \log(h[\vec{w}](\vec{x}_k)) + (1 - c_k) \log(1 - h[\vec{w}](\vec{x}_k))$$

# Gradient of the Error Function

Consider the **gradient** of the error function:

$$\nabla E(\vec{w}) = \left( \frac{\partial E}{\partial w_0}(\vec{w}), \dots, \frac{\partial E}{\partial w_n}(\vec{w}) \right) = \sum_{k=1}^p (h[\vec{w}](\vec{x}_k) - c_k) \cdot \tilde{\mathbf{x}}_k$$

## Fact 1

*If  $\nabla E(\vec{w}) = \vec{0} = (0, \dots, 0)$ , then  $\vec{w}$  is a global minimum of  $E$ .*

This follows from the fact that  $E$  is convex.

Using the squared error with the logistic sigmoid would lead to a non-convex error with several minima!

# Logistic Regression – Learning

## Gradient Descent:

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## Proposition

*For sufficiently small  $\varepsilon > 0$ , the sequence  $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \dots$  converges (in a component-wise manner) to the global minimum of the error function  $E$ .*

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We have already trained our logistic regression model, i.e., we have a vector of weights  $\vec{w} = (w_0, w_1, \dots, w_n)$ .

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To decide whether a given  $\vec{x}$  belongs to the class 1 we use  $h[\vec{w}]$  as a Bayes classifier: Assign  $\vec{x}$  to the class 1 iff  $h[\vec{w}](\vec{x}) \geq 1/2$ .

Other thresholds can also be used depending on the application and properties of the model. In such a case, given a threshold  $\xi \in [0, 1]$ , assign  $\vec{x}$  to the class 1 iff  $h[\vec{w}](\vec{x}) \geq \xi$ .

# Maximum Likelihood vs Cross-entropy (Dim 1)

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The following conditions are equivalent:

- ▶  $w_0, w_1$  minimize the binary cross-entropy  $E$
- ▶  $w_0, w_1$  maximize the likelihood (i.e., the “probability”) of generating the correct values  $c_1, \dots, c_p$  using the above described Bernoulli trials (i.e., that  $c'_k = c_k$  for all  $k = 1, \dots, p$ )

Note that the above equivalence is a property of the cross-entropy and is not dependent on the “implementation” of  $h[w_0, w_1](x_k)$  using the logistic sigmoid.