# 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).

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.

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- 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 understanding of 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.

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

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### Arthur Samuel, 1959

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

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 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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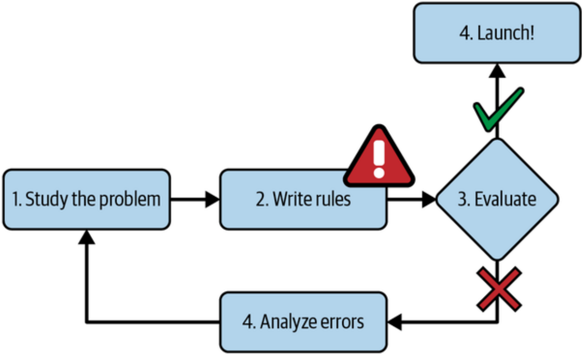
In the context of customer behavior:

- 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?

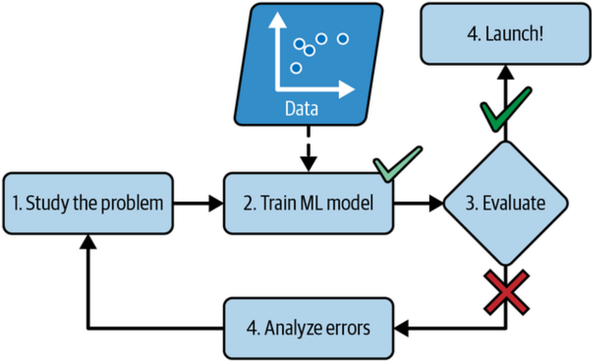
- Examine what spam mails typically contain: Specific words ("Viagra"), sender's address, etc.
- Write down a rule-based system that detects specific features.
- Test the program on new emails and (most probably) go back to look for more spam features.



# Comparison of Programming and Learning

The machine learning way:

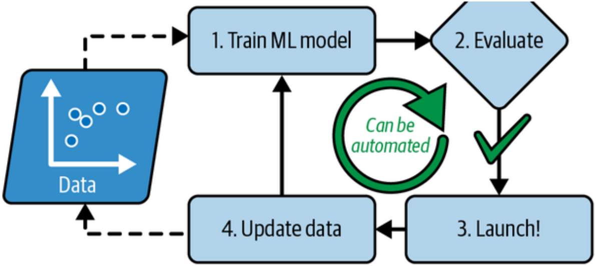
- Study the problem and collect lots of emails, labeling them spam or ham.
- Train a machine learning model that reads an email and decides whether it's spam or ham.
- Test the model and (most probably) go back to collect more data and adjust the model.



# ML Solutions are Adaptive

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

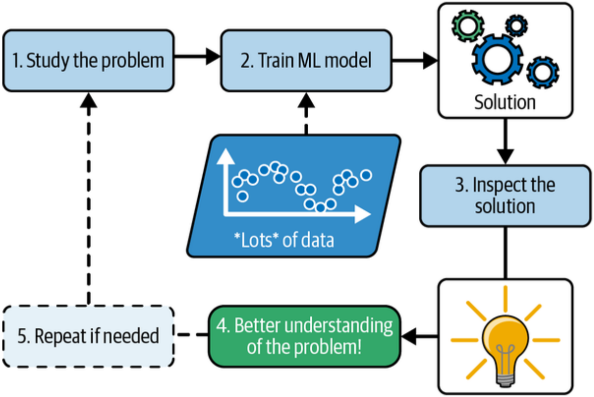
ML systems can be adjusted to new situations by retraining on new data (unless the data becomes ugly).



# 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.

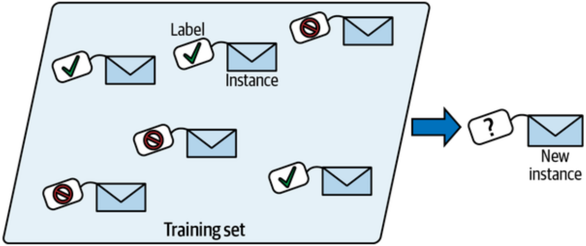
In summary, machine learning offers innovative solutions and adaptability for today's complex and ever-changing problems, (sometimes) providing insights beyond the reach of traditional approaches.

# Types of Learning

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

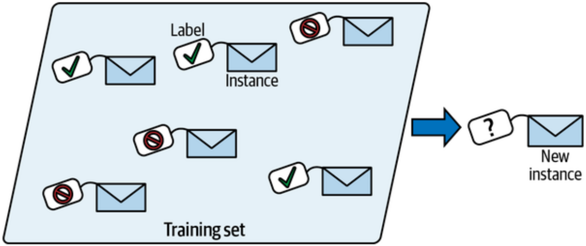
- Supervised learning
- Unsupervised learning
- Semi-supervised learning
- Self-supervised learning
- Reinforcement learning

# Supervised Learning




Labels are available for all input data.

# Supervised Learning

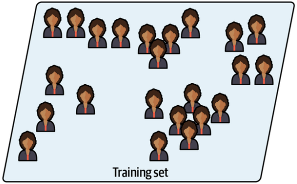


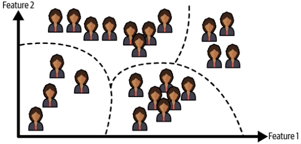

Labels are available for all input data.

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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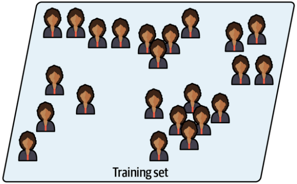


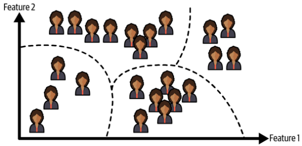


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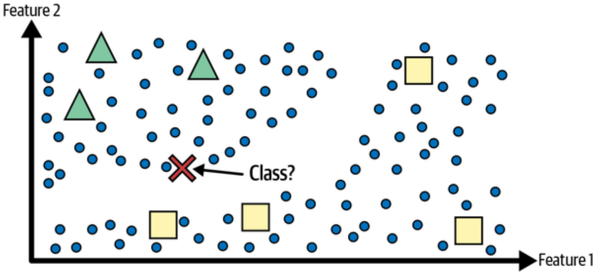
Typical unsupervised learning tasks are

- *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

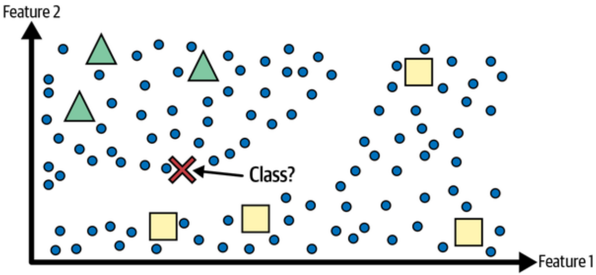
  (e.g., market basket mining where associations between various types of goods are being learned from the behavior of customers)
- *Dimensionality reduction* reduce high-dimensional data to few dimensions (e.g., images to few image features)

# Semi-Supervised Learning




Labels for some data.

# Semi-Supervised Learning

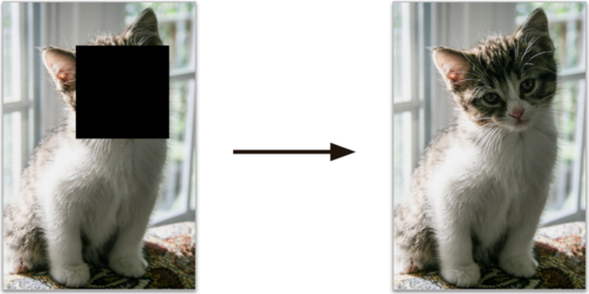



Labels for some data.

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

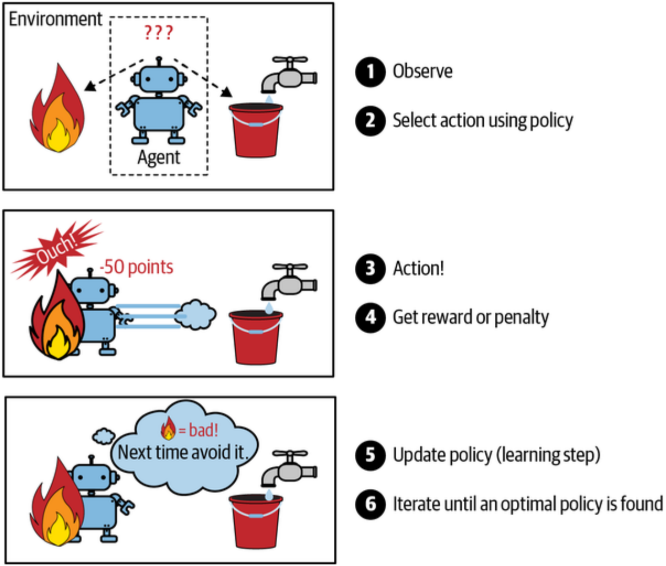


Generate labels from (unlabeled) inputs.

The goal is to learn typical features of the data.

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

# Reinforcement Learning




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
  - Currently extended to multimodal versions (text, image, sound)

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- Various "table" data processing in finance, management, etc.
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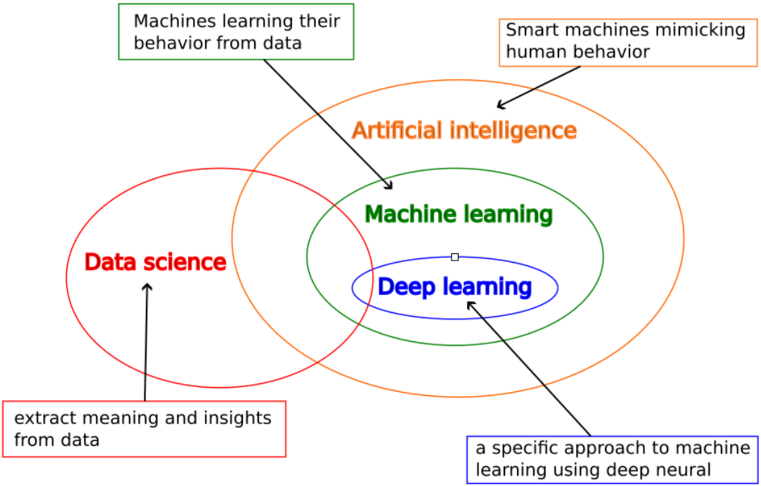
  - Essential but not fancy
- Game playing: More fancy than useful, learning models beating humans in several difficult games.

# ML in Context



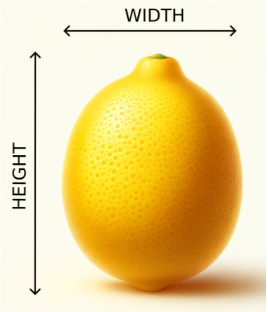
# Supervised Learning

# Example - Fruit Recognition

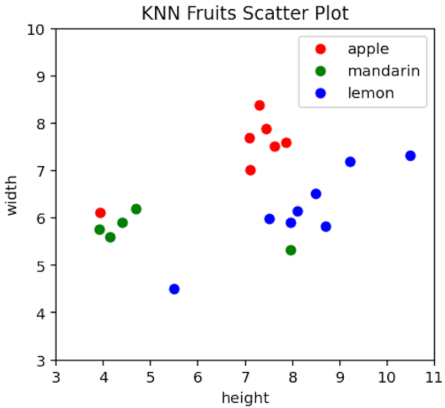
**The goal:** Create an automatic system for fruit recognition, concretely apple, lemon, and mandarin.

**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



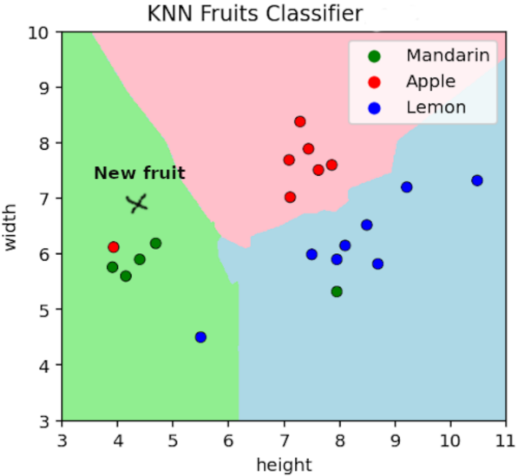

Use similarity to solve the problem.

| | 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 |

# KNN Classification

Given a new fruit.
What is it?

Find five closest examples




Where is the machine learning?

# KNN Classification

Given a new fruit.
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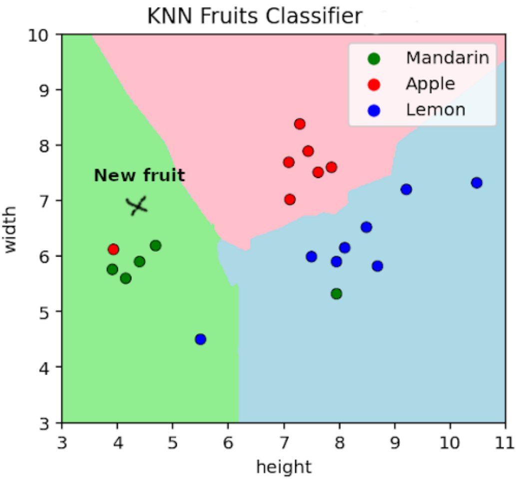
Find five closest examples

Among the five closest:

- $M = 4$ mandarins
- $A = 1$ apples
- $L = 0$ lemons

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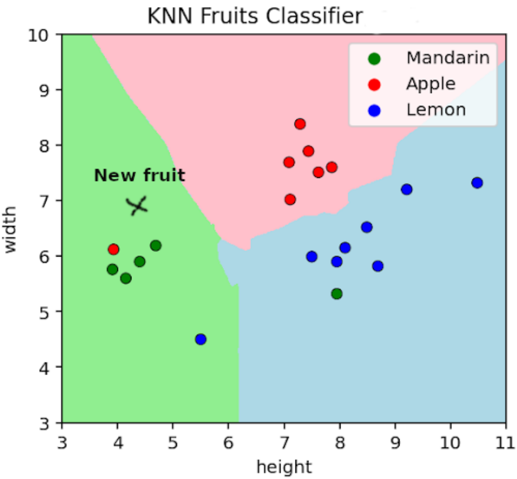
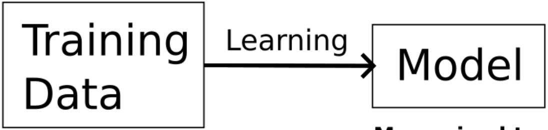
It is a **mandarin**!




Where is the machine learning?

# Learning in Fruit Classification with KNN

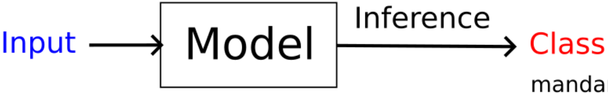
**Learning:**




A table with dimensions of fruits + correct classes

**Memorized traing data** +
the constant K +
the distance measure d

**Inference:**




A fruit dimensions

mandarin or
lemon or
apple

# Fruit Classification Algorithm

**Input:** A fruit $F$ with dimensions *height*, *width*
**Output:** *mandarin*, *lemon*, *apple*

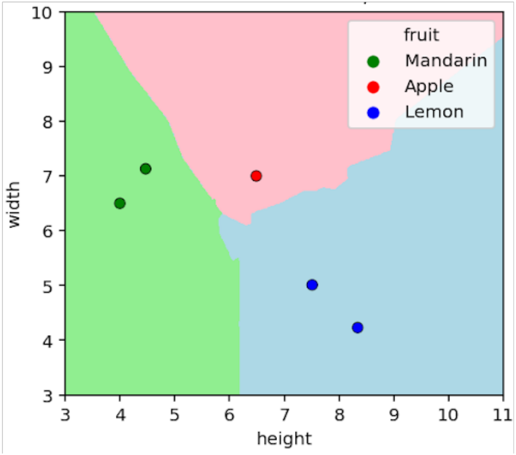
Find $K$ examples $\{E_1, \ldots, E_K\}$ in the dataset whose dimensions are closest to the dimensions of the fruit $F$
Count the number of examples of each class in $\{E_1, \ldots, E_K\}$
    $M$ mandarins in $\{E_1, \ldots, E_K\}$
    $L$ lemons in $\{E_1, \ldots, E_K\}$
    $A$ apples in $\{E_1, \ldots, E_K\}$
**if** $M \geq L$ and $M \geq A$ **then return** *mandarin*
**else if** $L \geq A$ **then return** *lemon*
**else return** *apple*
**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!!

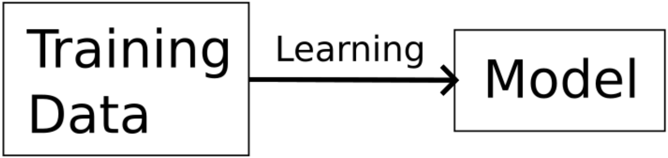
# K Nearest Neighbors

…on ideal data

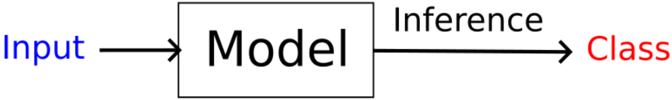
# Learning and Inference

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

$$\begin{array}{cccc|c} x_{11} & x_{12} & \cdots & x_{1n} & c_1 \\ x_{21} & x_{22} & \cdots & x_{2n} & c_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{p1} & x_{p2} & \cdots & x_{pn} & c_p \end{array}$$

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Formally, we define **training dataset**

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

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

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

# KNN: Learning

Consider the training set:

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

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 $\mathcal{T} = \{(\vec{x}_k, c_k) \in \mathbb{R}^n \times C \mid k = 1, \ldots, p\}$, 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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For $d$, consider Euclidean distance, but different norms may also be used to define different distance measures.

**Input:** A vector $\vec{z} = (z_1, \ldots, z_n) \in \mathbb{R}^n$
**Output:** A class from $C$

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

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

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 $d$.

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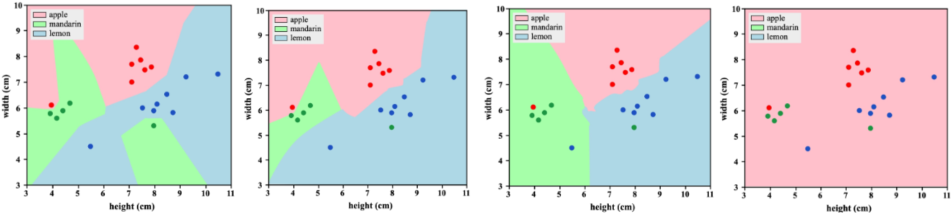
Note that different settings of $K$ lead to different classifiers (for the same $d$):



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- Deal with issues in the data
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  - 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 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.

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  - 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.

# In Practice

. . . to get an efficient solution:

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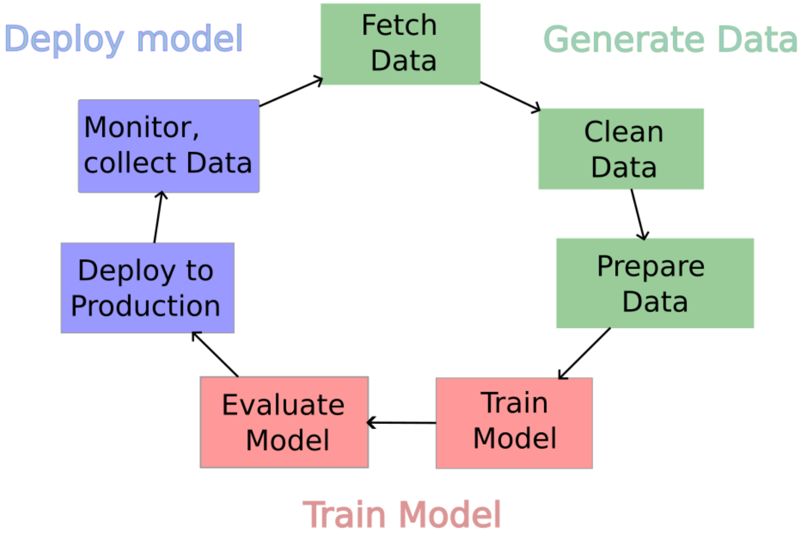
. . . but first, let us see the whole machine learning pipeline.

# Machine Learning Pipeline



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  In our example, the data is possibly small (just tables with results of tests). But for other diagnoses, you may include huge amounts of data from MRI, CT, etc. Then, the collection itself might be a serious technical problem.

- 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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**Data Separation**
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 $m << n$.

  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

Now the dataset has been cleaned; we may train a model.

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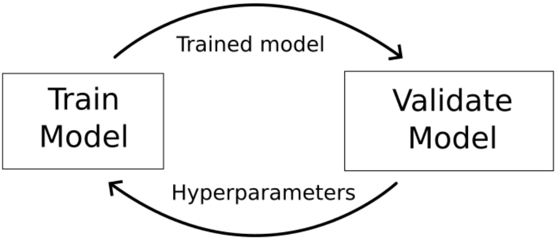
Before training, we should split the dataset into

- *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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| 012 | 232 | 33.5 | 0 | 10.7 |
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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

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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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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:**

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

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

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

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

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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

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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 | IQ scores, Celsius temperature, NPS data, etc. | Height, weight, income, etc. |

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- *Continuous*

  An uncountably infinite range of values, typically 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

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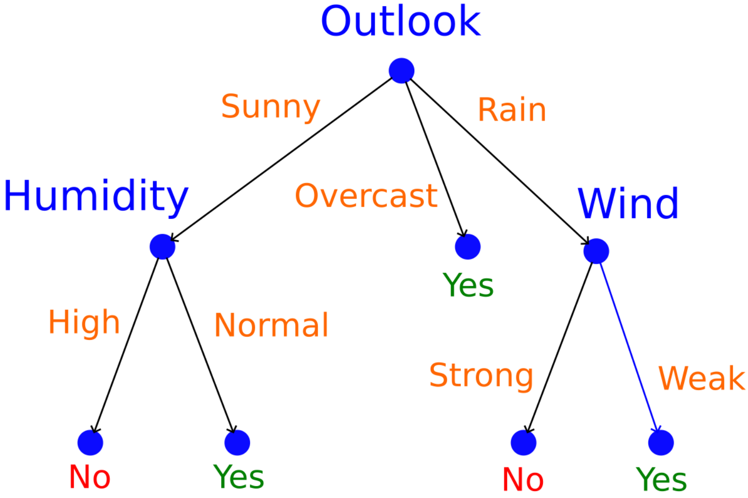
- We will consider the ID3 algorithm.
  Quinlan, 1979
- Various adjustments that appear in C4.5, CART, etc.

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



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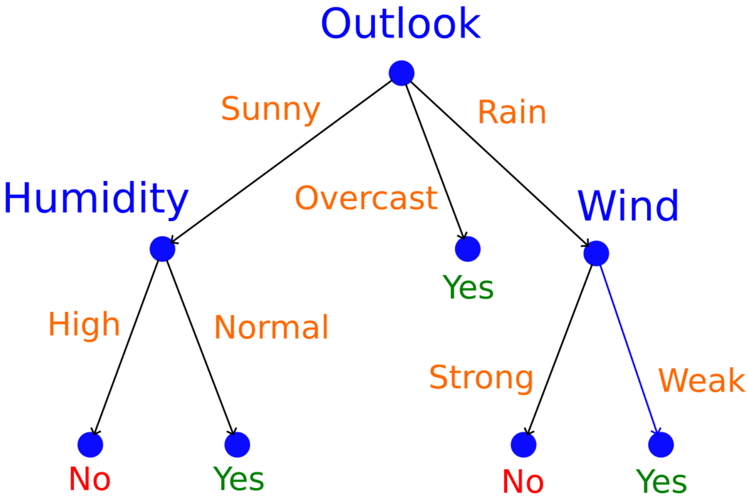


How do we obtain such a tree based on experience/data?

# Learning Decision Trees

Consider data represented as follows:

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

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

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

Given $\vec{x}$ and an attribute $A_k$ we denote by $A_k(\vec{x})$ the value $x_k$ of the attribute $A_k$ in $\vec{x}$.

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- A finite set of *attributes* $\mathcal{A} = \{A_1, \ldots, A_n\}$.
- 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 $A \in \mathcal{A}$.

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

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

Given $\vec{x}$ and an attribute $A_k$ we denote by $A_k(\vec{x})$ the value $x_k$ of the attribute $A_k$ in $\vec{x}$.

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:

$$A_1 = \textit{Outlook}, A_2 = \textit{Temperature}, A_3 = \textit{Humidity}, A_4 = \textit{Wind}$$

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  - $V(A_2) = \{\textit{Hot}, \textit{Mild}, \textit{Cool}\}$
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- Consider

$$\vec{x} = (\mathit{Overcast}, \mathit{Hot}, \mathit{Normal}, \mathit{Weak}) \in V(A_1) \times V(A_2) \times V(A_3) \times V(A_4)$$

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- $C = \{\textit{Yes}, \textit{No}\}$

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Consider (directed, rooted) *trees* $\mathcal{T} = (T, E)$ where $T$ is a set of nodes and $E \subseteq T \times T$ is a set of directed edges.

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A *decision tree* is

- a tree $\mathcal{T} = (T, E)$ where
- each leaf $\tau \in T_{leaf}$ is assigned a class $C(\tau) \in C$,
- each internal node $\tau \in T_{int}$ is assigned an attribute $A(\tau) \in \mathcal{A}$,
- 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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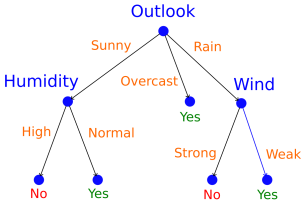
**Inference:** Given an input $\vec{x}$, we traverse the tree from the root to a leaf, always choosing edges labeled with values of attributes from $\vec{x}$. The output is the class labeling the leaf.

# Example

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

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

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




$$C(z_1) = C(z_3) = No,\ C(z_2) = C(z_4) = Yes$$

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

$$V(O, H) = Sunny,\ V(O, z_3) = Overcast,\ V(O, W) = Rain$$
$$V(H, z_1) = High,\ V(H, z_2) = Normal$$
$$V(W, z_4) = Strong,\ V(W, z_5) = Weak$$

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

# Training Dataset

Consider a *training dataset*

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

Here $\vec{x}_k \in V(A_1) \times \cdots \times V(A_k)$ 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 |

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

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

  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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  - for every $v \in V(A)$ introduce an edge $(\tau, \tau_v)$ assigned $v$.

**function** ID3(dataset $\mathcal{D}$, attribute set $\mathcal{A}$)
    Create a root node $\tau$ for the tree
    **if** $\mathcal{D} = \emptyset$ **then**
        Return the single node $\tau$ assigned with a default class.
    **else if** all examples in $\mathcal{D}$ are of the same class $c$ **then**
        Return the single-node tree, where $\tau$ is assigned $c$
    **else if** set of attributes $\mathcal{A}$ is empty **then**
        Return the single-node tree where $\tau$ is assigned the most common class in $\mathcal{D}$
    **else**
        Choose attribute $A \in \mathcal{A}$ *best classifying* examples in $\mathcal{D}$.
        Set the decision attribute for $\tau$ to $A$
        **for** each value $v \in D(A)$ **do**
            Compute a decision tree ID3($\mathcal{D}_v, \mathcal{A} \setminus \{A\}$) with root $\tau_v$,
            add a new edge $(\tau, \tau_v)$ assigned $v$.
        **end for**
    **end if**
**return** $\tau$
**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 define the *entropy* of $\mathcal{D}$ by

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

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

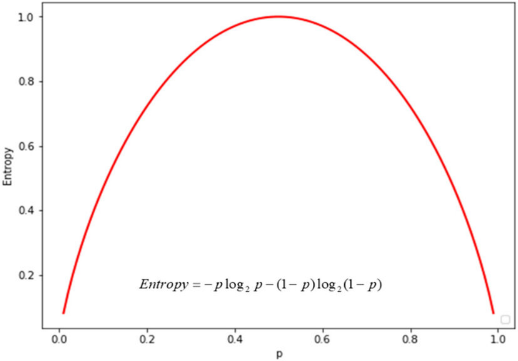
$$Gain(\mathcal{D}, A) = Entropy(\mathcal{D}) - \sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Entropy(\mathcal{D}_v)$$

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

# Information Gain

The intuition behind information gain:

- Consider $C = \{0, 1\}$ and $p$ the proportion of examples of class 1. $p$ measures the "uncertainty" of the class:



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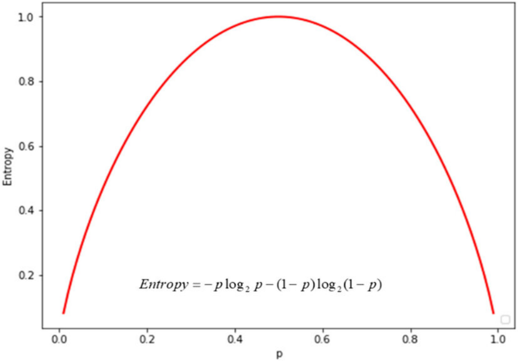


- $\sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Entropy(\mathcal{D}_v)$ is weighted uncertainty of classes in each $\mathcal{D}_v$ (weighted by the relative size of $\mathcal{D}_v$).

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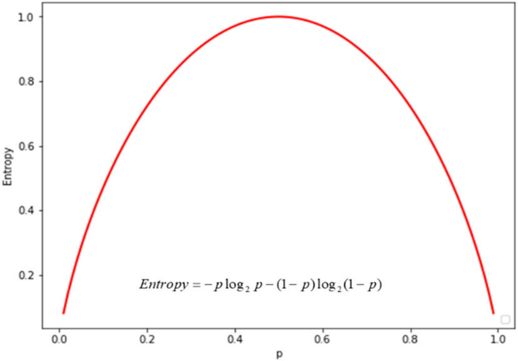


- $\sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Entropy(\mathcal{D}_v)$ is weighted uncertainty of classes in each $\mathcal{D}_v$ (weighted by the relative size of $\mathcal{D}_v$).
- $Gain(\mathcal{D}, A)$ measures reduction in uncertainty of classes by splitting $\mathcal{D}$ according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

# Gini Impurity

- We define *Gini impurity* of $\mathcal{D}$ by

$$Gini(\mathcal{D}) = 1 - \sum_{c \in C} p_c^2$$

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$$Gini(\mathcal{D}) = 1 - \sum_{c \in C} p_c^2$$

- 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.

# Example

Consider our tennis example (see the table).

- Consider the whole dataset $\mathcal{D}$.
  - $p_{Yes} = 9/14$
  - $p_{No} = 5/14$
  - $Gini(\mathcal{D}) = 1 - (9/14)^2 - (5/14)^2 = 0.45918$

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  - $Gini(\mathcal{D}) = 1 - (9/14)^2 - (5/14)^2 = 0.45918$
- For $A = Outlook$ we get
  - $Gini(\mathcal{D}_{Sunny}) = 1 - (2/5)^2 - (3/5)^2 = 0.48$
  - $Gini(\mathcal{D}_{Overcast}) = 1 - 1^2 - 0^2 = 0$
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  Thus

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

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

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 attribude after *Sunny* in *Outlook* is *Humidity*.

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

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

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

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

# 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.

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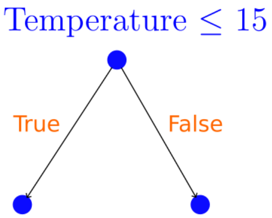
$A$ is a numerical attribute that can take any value in an interval, such as temperature, size, time, etc.

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* $H \in \mathbb{R}$,
- there are two edges $e_{\text{true}}, e_{\text{false}}$ from $\tau$,
- $e_{\text{true}}$ labeled with True and $e_{\text{false}}$ labeled with False.

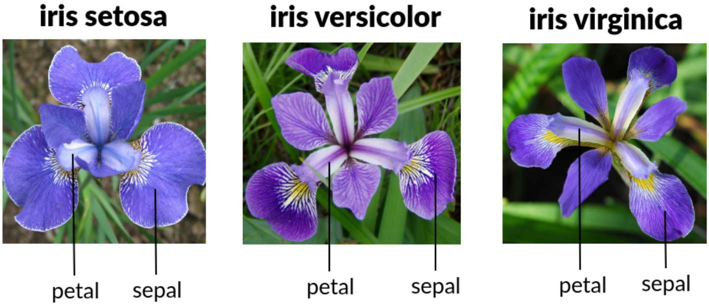
During inference, when considering an example $\vec{x}$ in the node $\tau$,

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




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




**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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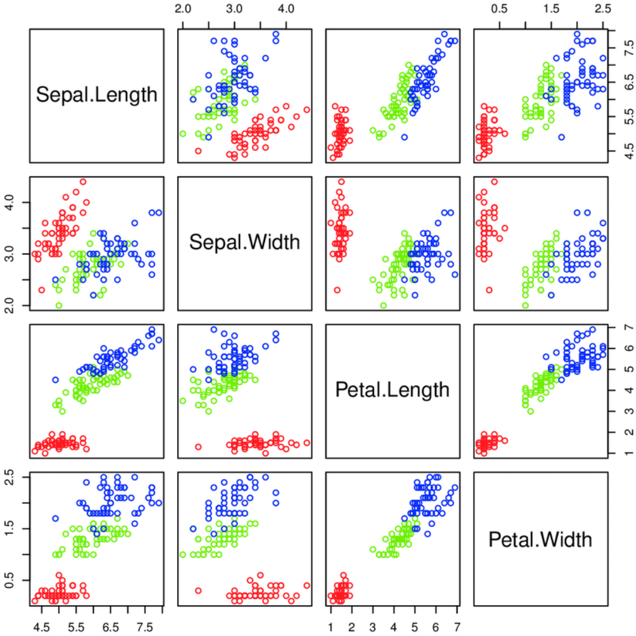
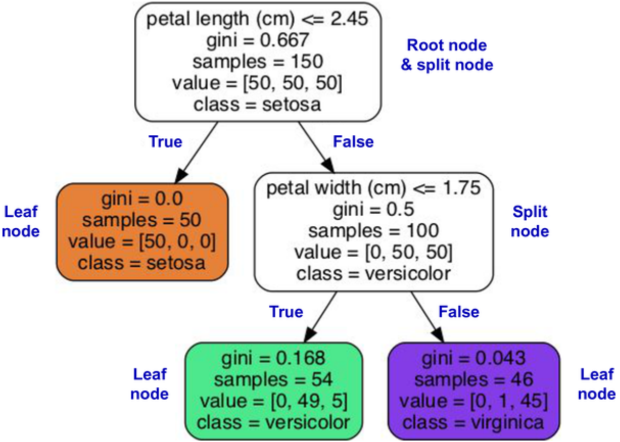
| 4.4 | 2.9 | 1.4 | 0.2 | Setosa |
| 6.0 | 3.4 | 4.5 | 1.6 | Versicolor |
| 5.1 | 3.5 | 1.4 | 0.2 | Setosa |
| 6.6 | 3.0 | 4.4 | 1.4 | Versicolor |
| 5.9 | 3.2 | 4.8 | 1.8 | Versicolor |
| 5.6 | 2.8 | 4.9 | 2.0 | Virginica |
| ... | | | | |

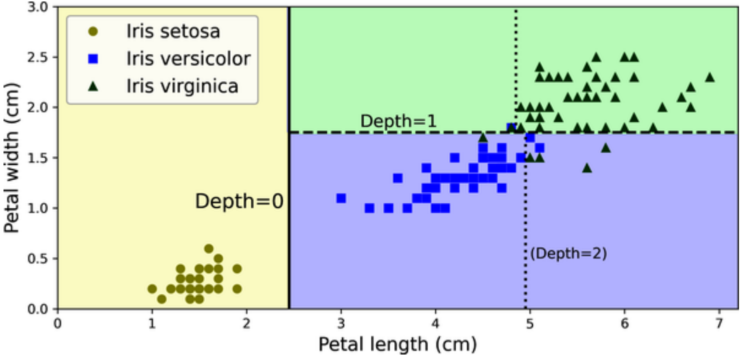
# Iris Example



# Iris Example - Decision Tree



# Iris Example - Decision Tree Boudaries




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

# Attribute Importance Computation

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

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

# Decision Trees

Practical Issues

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

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

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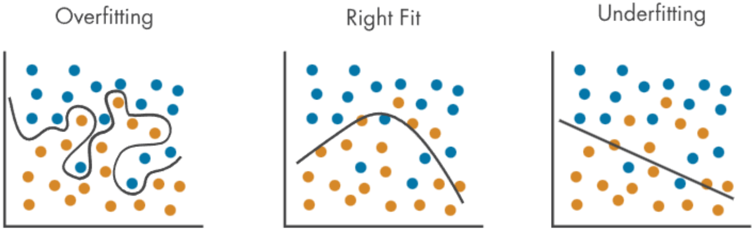
For small $|\mathcal{D}_a|$ (say $\leq 1000$) we have small $|\mathcal{D}_a|/|\mathcal{D}|$

For not so small $\mathcal{D}_a$ we have $Gini(\mathcal{D}_a) \approx 0$.

In both cases, the impurity decrease is very small.

# Model Tuning - Over/Under Fitting

The behavior of the model on the training set:



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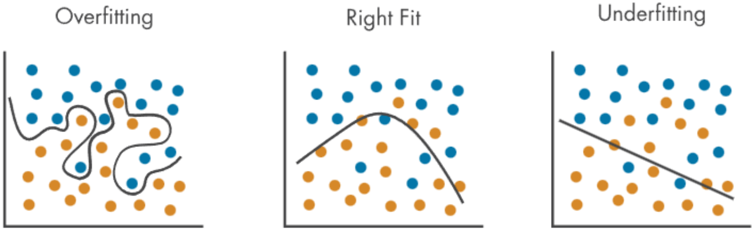


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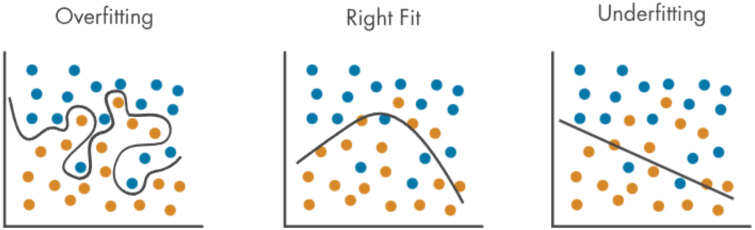


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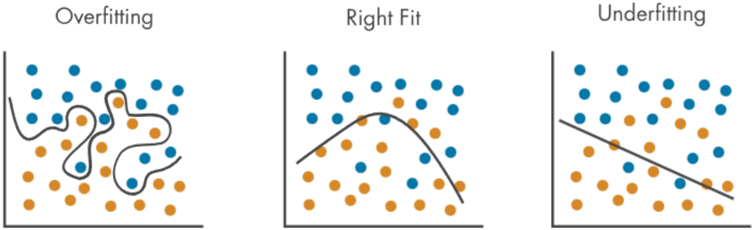


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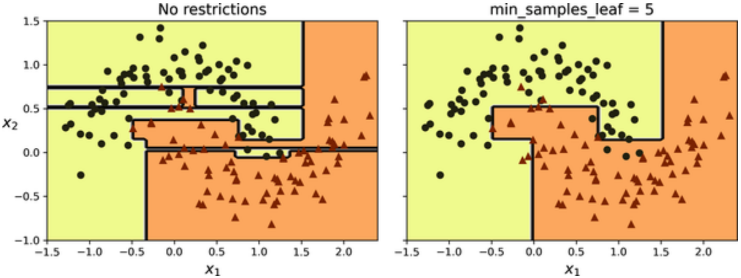
- The middle one seems good (but still needs to be tested on fresh data).

# Model Tuning - Overfitting in Decision Trees

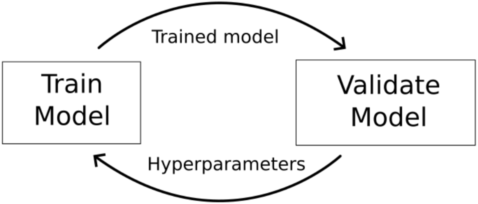



See the overfitting on the left and the "nice" model on the right.

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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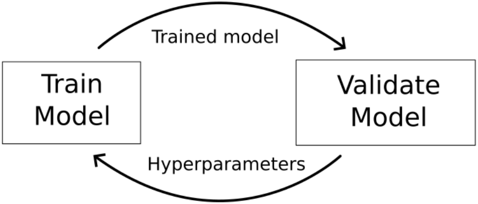


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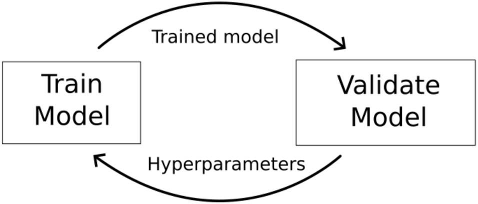


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What to observe? In the case of decision trees, one should observe the difference between performance measures (e.g., classification accuracy) on the training and validation sets.

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-Prunning - Hyperparamaters

Hyperparameters controlling the size of the tree:

- Maximum depth - do not grow the tree beyond the max depth

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

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  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.

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Train $\mathcal{T}$ to maximum fit on the *training dataset.*<br>
**while** true **do**<br>
    $Err[\mathcal{T}] \leftarrow$ the error of $\mathcal{T}$ on the validation set.<br>
    **for** $\tau \in T_{int}$ **do**<br>
        $Err[\mathcal{T}_{-\tau}] \leftarrow$ the error of $\mathcal{T}_{-\tau}$ on the validation set.<br>
    **end for**<br>
    **if** $Err[\mathcal{T}] \leq \min\{Err[\mathcal{T}_{-\tau}] \mid \tau \in T_{int}\}]$ **then return** $\mathcal{T}$<br>
    **else**<br>
        $\mathcal{T} \leftarrow argmin\{Err[\mathcal{T}_{-\tau}] \mid \tau \in T_{int}\}$<br>
    **end if**<br>
**end while**

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

# 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.
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- Using cost complexity measure: Evaluate trees not only based on the classification error but also based on their size.

  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.

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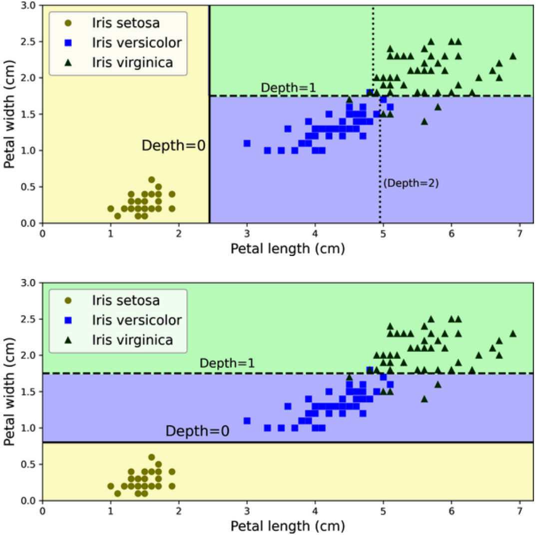
A solution is to train an ensemble of many decision trees and then use majority voting for classification.

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

# Iris - Illustration

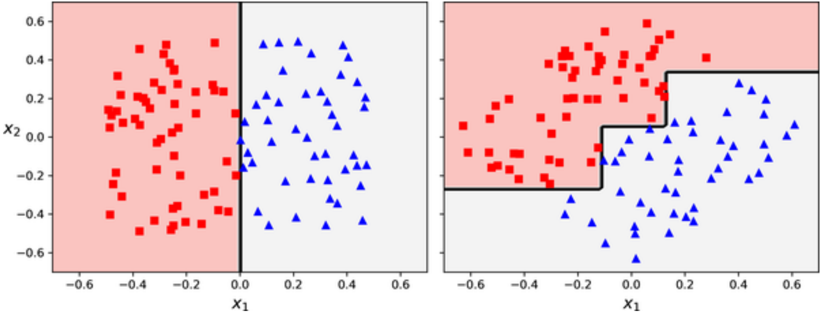



Decision trees trained on the Iris dataset.

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

# Axis Sensitivity

The decision makes divisions along particular axes:

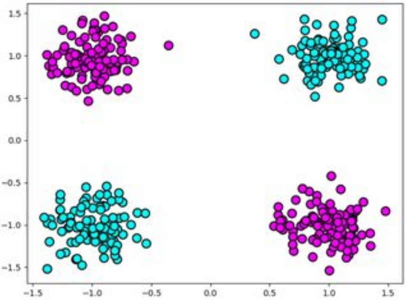



That is, rotated data may result in a completely different model.

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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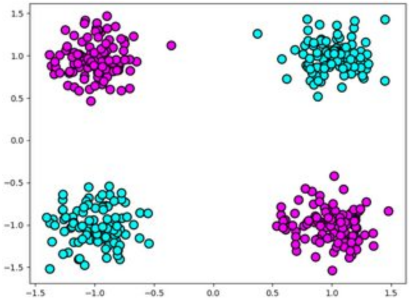
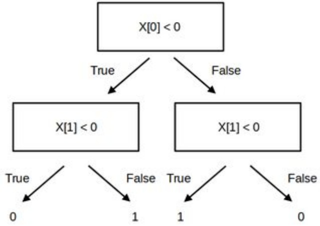



An ideal decision tree would look like this:



# Attempts at Training on XOR

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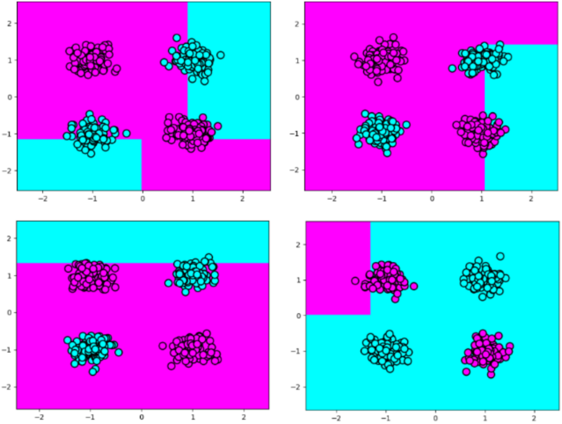

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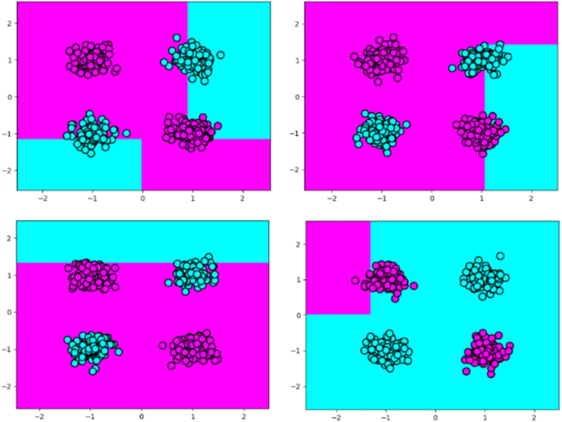
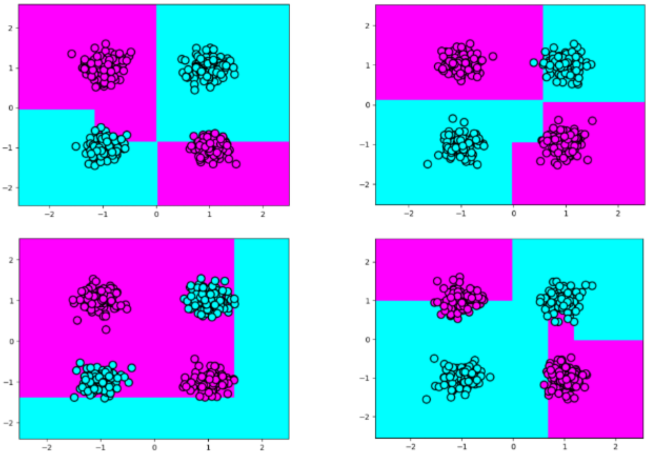


The problem: Both information gain and decrease in impurity consider only the relationship of a *single* attribute and the class.

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.
- Instability: Small data variations can result in very different trees. This is mitigated in ensemble methods.
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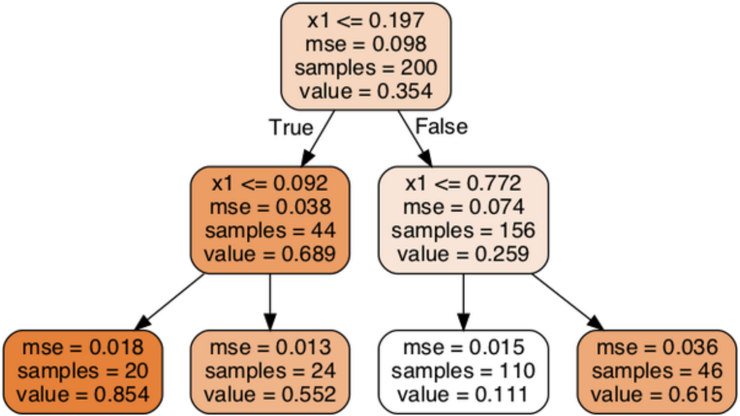
- Learning optimal trees is NP-complete: Heuristic algorithms like greedy algorithms are used, which do not guarantee globally optimal trees. Ensemble methods can help.

# 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.

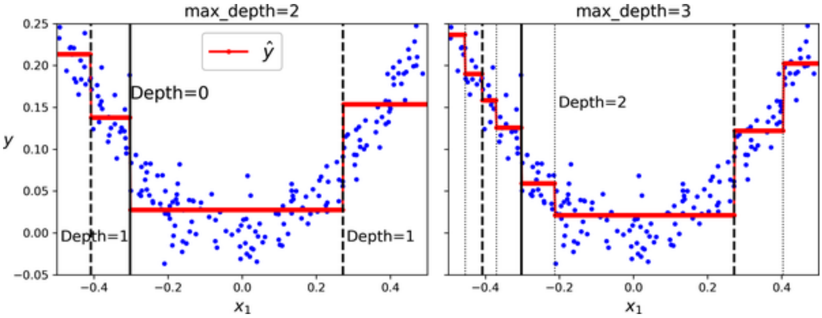
# Comment on Regression Trees

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. We get to this notion later in connection with linear models and neural networks.

# 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? We will answer this question later once we master the mean-squared error.

# Probabilistic Classification

# Probabilistic Classification – Idea

Imagine that

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- it is black, approx. 25 cm long and has a rather yellow beak.

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Here *probably* means that out of my extensive catalog of four kinds of birds that I can recognize, "blackbird" gets the highest degree of belief based on *features* of this particular bird.

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

# Basic Discrete Probability Theory

- A finite or countably infinite set $\Omega$ of *possible outcomes*, $\Omega$ is called *sample space*.

  Experiment: Roll one dice once. Sample space: $\Omega = \{1, \ldots, 6\}$

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- Each element $\omega$ of $\Omega$ is assigned a "probability" value $f(\omega)$, here $f$ must satisfy
  - $f(\omega) \in [0, 1]$ for all $\omega \in \Omega$,
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  If the dice is fair, then $f(\omega) = \frac{1}{6}$ for all $\omega \in \{1, \ldots, 6\}$.

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- An *event* is any subset $E$ of $\Omega$.
- The *probability* of a given event $E \subseteq \Omega$ is defined as

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  Let $E$ be the event that an odd number is rolled, i.e., $E = \{1, 3, 5\}$. Then $P(E) = \frac{1}{2}$.
- 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

$$P(A \mid B) = P(A \cap B)/P(B)$$

(We assume that $B$ is all and only information known.)

A fair dice: what is the probability that 3 is rolled assuming that an odd number is rolled? ... and assuming that an even number is rolled?

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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

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

# Random Variables and Random Vectors

- A *random variable* $X$ is a function $X : \Omega \to \mathbb{R}$.
  A dice: $X : \{1, \dots, 6\} \to \{0, 1\}$ such that $X(n) = n \mod 2$.
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  We use $X = (X_1, \ldots, X_d)$ 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

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

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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$$\begin{aligned} P(red, circle) &= P(X_{color} = red, X_{shape} = circle) \\ &= P(red, circle, \mathbf{1}) + P(red, circle, \mathbf{0}) \\ &= 0.2 + 0.05 = 0.25 \end{aligned}$$

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$$P(red) = 0.2 + 0.02 + 0.05 + 0.3 = 0.57$$

Thus also, all conditional probabilities can be computed:

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

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- Let $X$ be the random vector describing $n$ features of a given instance, i.e., $X = (X_1, \ldots, X_n)$
  - Denote by $\vec{x} \in \mathbb{R}^n$ values of $X$,
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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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We are given a fruit of a diameter of $5cm$ that weighs $40g$.

The Bayes classifier compares $P(Y = \mathbf{1} \mid X = (40g, 5cm))$ with $P(Y = \mathbf{0} \mid X = (40g, 5cm))$ 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.

# Bayes Classifier

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## 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 $P(Y = \mathbf{1} \mid X = \vec{x})$ ?
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Given no other assumptions, this requires a table showing the probability of the category $\mathbf{1}$ for each possible feature vector $\vec{x}$.

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 $P$

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Part of the data table:

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All data with $X_1 = 1$, $X_2 = 0$, $X_3 = 1$:

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The probability table and the necessary data are typically too large!

Concretely, if all $X_1, \ldots, X_n$ 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)

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

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Proof.

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

□

# 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:

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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

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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).

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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 $\vec{x} = (x_1, \ldots, x_n)$ and $y \in \{\mathbf{0}, \mathbf{1}\}$ we **assume**:

$$P(X = x \mid Y = y) = P(X_1 = x_1, \cdots, X_n = x_n \mid Y)$$
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  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 $y \in \{\mathbf{0}, \mathbf{1}\}$.

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

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| **0** | 1 | 0 | 1 |
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| **1** | 0 | 0 | 0 |
| **0** | 1 | 1 | 1 |

$\bar{P}(X_1 = 1 \mid Y = \mathbf{1}) = 1/3$ $\bar{P}(X_1 = 1 \mid Y = \mathbf{0}) = 2/3$
$\bar{P}(X_2 = 1 \mid Y = \mathbf{1}) = 1/3$ $\bar{P}(X_2 = 1 \mid Y = \mathbf{0}) = 1/3$
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# Naive Bayes – Example

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 |
| $\bar{P}(medium \mid Y)$ | 0.1 | 0.2 |
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Denote $\vec{x} = (medium, red, circle)$.

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

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

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

| | $Y = \mathbf{1}$ | $Y = \mathbf{0}$ |
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$$\doteq 0.5 \cdot 0.2 \cdot 0.3 \cdot 0.3 \,/\, P(X = \vec{x}) = 0.009/P(X = \vec{x})$$

(Note that we used the estimates $\bar{P}$ of $P$ to finish the computation above.)
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 **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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- $\ell_y$ = number of samples with $Y = y$

**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 | **1** |
| large | red | circle | **1** |
| small | red | triangle | **0** |
| large | blue | circle | **0** |

Estimated probabilities:

| | $Y = \mathbf{1}$ | $Y = \mathbf{0}$ |
|---|---|---|
| $\bar{P}(Y)$ | 0.5 | 0.5 |
| $\bar{P}(small \mid Y)$ | 0.5 | 0.5 |
| $\bar{P}(medium \mid Y)$ | 0 | 0 |
| $\bar{P}(large \mid Y)$ | 0.5 | 0.5 |
| $\bar{P}(red \mid Y)$ | 1 | 0.5 |
| $\bar{P}(blue \mid Y)$ | 0 | 0.5 |
| $\bar{P}(green \mid Y)$ | 0 | 0 |
| $\bar{P}(square \mid Y)$ | 0 | 0 |
| $\bar{P}(triangle \mid Y)$ | 0 | 0.5 |
| $\bar{P}(circle \mid Y)$ | 1 | 0.5 |

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

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

# Smoothing

- To account for estimation from small samples, probability estimates are adjusted or *smoothed*.

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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

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

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

# Laplace Smoothing Example

- Assume training set contains 10 samples of category **1**:
  - 4 small
  - 0 medium
  - 6 large

# Laplace Smoothing Example

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

# Continuous Features

$\Omega$ may be (potentially) continuous, $X_i$ may assign a continuum of values in $\mathbb{R}$.

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- The probabilities are computed using *probability density* $p : \mathbb{R} \to \mathbb{R}^+$.
  A random variable $X : \Omega \to \mathbb{R}^+$ has a density $p : \mathbb{R} \to \mathbb{R}^+$ if for every interval $[a, b]$ we have
  $$P(a \leq X \leq b) = \int_a^b p(x)dx$$
  Usually, $P(X_i \mid Y = y)$ is used to denote the *density* of $X_i$ conditioned on $Y = y$.

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  Usually, $P(X_i \mid Y = y)$ is used to denote the *density* of $X_i$ conditioned on $Y = y$.
- The densities $P(X_i \mid Y = y)$ 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

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

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- Tends to work well despite rather a strong assumption of conditional independence of features.

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  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.
- Missing values are easy to deal with (simply average overall missing values in feature vectors).

# Bayesian Networks (Basic Information)

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What if we return some dependencies?

(But now in a well-defined sense.)

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What if we return some dependencies?

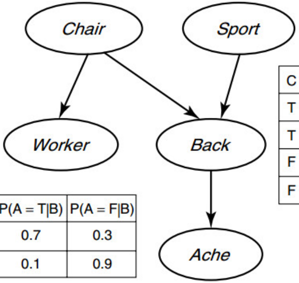
(But now in a well-defined sense.)

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 |




| C | P(W = T\|C) | P(W = F\|C) |
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| C | S | P(B = T\|C,S) | P(B = F\|C,S) |
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| B | P(A = T\|B) | P(A = F\|B) |
|---|---|---|
| T | 0.7 | 0.3 |
| F | 0.1 | 0.9 |

Now, e.g.,

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

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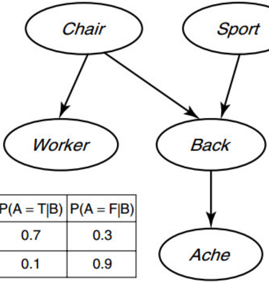


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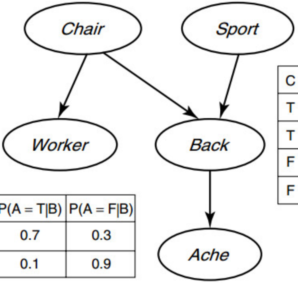


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$$P(C, S, W, B, A) = P(C) \cdot P(S) \cdot P(W \mid C) \cdot P(B \mid C, S) \cdot P(A \mid B)$$

Now, we may, e.g., infer the probability $P(C = T \mid A = T)$ 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 $Y, X_1, \ldots, X_n$ using a Bayesian network?

# Classifier Evaluation

# Classifier

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 |
| | 0 | FP | TN |

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$$\text{TP} = |\{k \mid h_k = 1 \wedge c_k = 1\}|$$

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Given a sample of 12 individuals, eight have cancer, and four are cancer-free.

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Assume that we have trained a classifier with the following results:

| **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 |
| **Predicted** | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 0 |
| **Result** | FN | FN | TP | TP | TP | TP | TP | TP | FP | TN | TN | TN |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Actual** | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 0 |
| **Predicted** | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 0 |
| **Result** | FN | FN | TP | TP | TP | TP | TP | TP | FP | TN | TN | TN |

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

# Terminology

- TP aka hit
- TN aka correct rejection
- FP aka type I error, false alarm, overestimation
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Usually, TP, TN, FP, and FN are used to denote the individual examples of a particular kind and the number of these examples.

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In what follows, we also use

- $\text{P} = \text{TP} + \text{FN}$ of all cases with the *actual* class 1
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- $\text{PP} = \text{TP} + \text{FP}$ of all cases with the *predicted* class 1
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Note that $\text{P} + \text{N} = \text{PP} + \text{PN}$ is the number of all cases.

# Terminology

- TP aka hit
- TN aka correct rejection
- FP aka type I error, false alarm, overestimation
- FN aka type II error, miss, underestimation

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There is a large number of derived metrics. We consider some of the most used in practice.

# Accuracy

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| **Actual condition** | **Predicted condition** | |
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The Accuracy is

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

# 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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The Accuracy is $91/100 > 0.9$. Pretty good, right?

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:

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

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

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

# Precision & Recall - Example

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- 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.

Which of the two is more important in medicine?

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:

$$\mathrm{F}_1 = \frac{2}{\mathrm{Recall}^{-1} + \mathrm{Precision}^{-1}} = \frac{2\mathrm{TP}}{2\mathrm{TP} + \mathrm{FP} + \mathrm{FN}}$$

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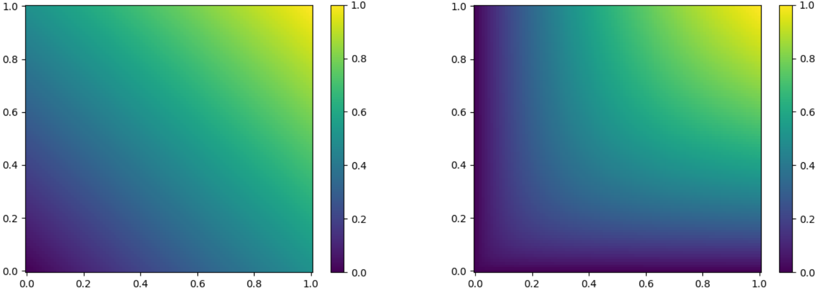
Compare the arithmetic (left) and harmonic (right) mean:




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

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Our imbalanced example:

| Actual | Predicted | |
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| | Pos | Neg |
| **Pos** | 1 | 9 |
| **Neg** | 0 | 90 |
| **Total** | 90 + 10 = 100 | |

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

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.

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Note that the standard definitions of Precision and Recall for binary classifiers reveal only part of the truth.

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

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

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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.

# $F_1$ Score

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- 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

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

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

# More Derived Metrics

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

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

How often is positive predicted positive?

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How often is negative predicted negative?

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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 $h_1, \ldots, h_p$ w.r.t. $c_1, \ldots, c_p$?

There are many possible metrics ...

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

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Formally,

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

| **Actual** | **Predicted** | | | | |
|---|---|---|---|---|---|
| | 1 | $\cdots$ | $j$ | $\cdots$ | $m$ |
| 1 | $M_{11}$ | $\cdots$ | $M_{1j}$ | $\cdots$ | $M_{1m}$ |
| $\vdots$ | $\vdots$ | | $\vdots$ | | $\vdots$ |
| $i$ | $M_{i1}$ | $\cdots$ | $M_{ij}$ | $\cdots$ | $M_{im}$ |
| $\vdots$ | $\vdots$ | | $\vdots$ | | $\vdots$ |
| $m$ | $M_{m1}$ | $\cdots$ | $M_{mj}$ | $\cdots$ | $M_{mm}$ |

# Example

| Actual | Predicted |
| --- | --- |
| big | big |
| big | big |
| small | big |
| medium | medium |
| big | small |
| big | big |
| small | small |
| small | small |
| medium | medium |
| medium | small |
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| small | small |
| medium | medium |
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| big | big |
| medium | small |
| small | medium |
| big | big |

| Actual | Predicted | | |
|---|---|---|---|
| | **big** | **medium** | **small** |
| **big** | 5 | 0 | 1 |
| **medium** | 0 | 2 | 2 |
| **small** | 1 | 1 | 3 |

Note that the diagonal counts the correctly classified samples.

The off-diagonal elements correspond to misclassified samples.

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

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

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

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

Precision[big] $= 5/6$

Precision[medium] $= 2/3$

Precision[small] $= 3/6$

Recall[big] $= 5/6$

Recall[medium] $= 2/4$

Recall[small] $= 3/5$

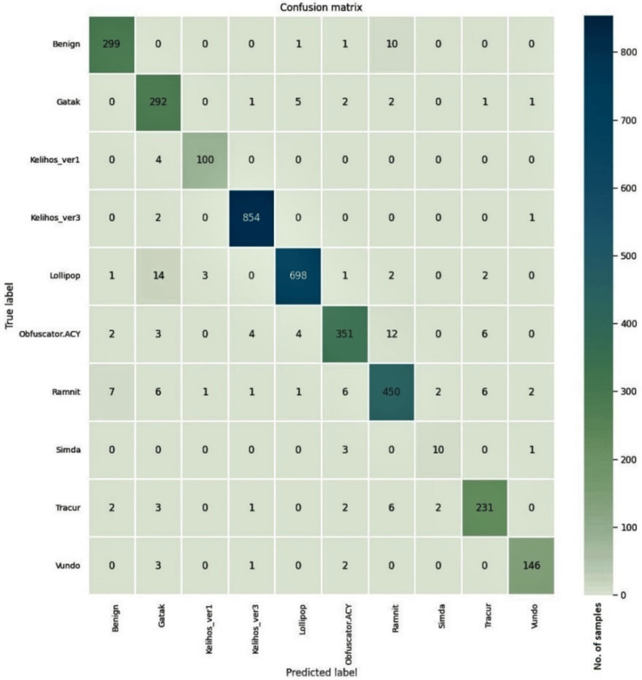
| Actual | Predicted | | |
|---|---|---|---|
| | **big** | **medium** | **small** |
| **big** | 5 | 0 | 1 |
| **medium** | 0 | 2 | 2 |
| **small** | 1 | 1 | 3 |

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

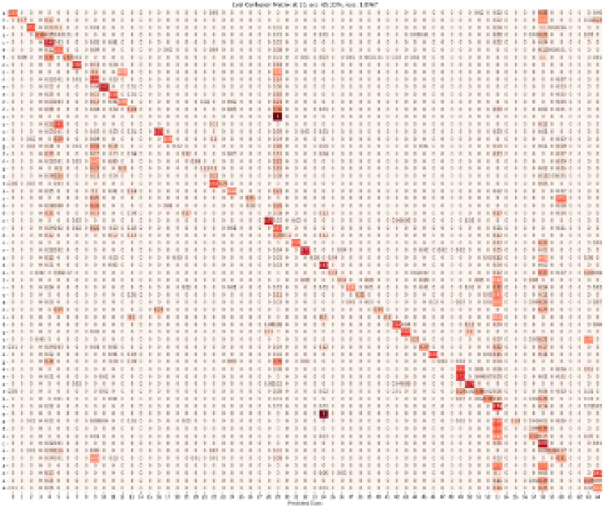
$F_1[\text{medium}] = 0.57$

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

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.



Confusion matrix
True label
Predicted label
No. of samples
Benign
Gatak
Kelihos_ver1
Kelihos_ver3
Lollipop
Obfuscator.ACY
Ramnit
Simda
Tracur
Vundo



Machine learning/data mining is needed to understand the matrix.

# Probabilistic Classifier Evaluation

# Binary Probabilistic Classifier

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

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Consider a classification dataset:

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

Here $\vec{x}_k$ is a vector of attributes/features and $c_k \in C$ for all $k$.

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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 $k$-the example $(\vec{x}_k, c_k)$.

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

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

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

# Probabilistic Classifier

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

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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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and

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and

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

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

# Thresholded Classifier Metrics

| **Index** | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Actual** | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 |
| **Predicted** | .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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| 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 |

For example, consider $T = 0.42$, then

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| T=0.42 | TP | TP | TP | TP | TP | FP | FP | TP | FN | TN | TN | TN |
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For example, consider $T = 0.42$, then

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

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

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

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

# Receiver Operating Characteristic (ROC)

Consider two metrics for a given $T$:

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

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

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

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

Observe that

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

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

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

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- $0.00 \leq T \leq 0.05$: TPR $= 1$ and FPR $= 1$

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- $0.00 \leq T \leq 0.05$: TPR $= 1$ and FPR $= 1$
- $0.05 < T \leq 0.10$: TPR $= 1$ and FPR $= 4/5$

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- $0.36 < T \leq 0.42$: TPR $= 6/7$ and FPR $= 2/5$

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- $0.36 < T \leq 0.42$: TPR $= 6/7$ and FPR $= 2/5$
- $0.42 < T \leq 0.43$: TPR $= 5/7$ and FPR $= 2/5$

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- $0.43 < T \leq 0.48$: TPR $= 5/7$ and FPR $= 1/5$

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- $0.48 < T \leq 0.66$: TPR $= 5/7$ and FPR $= 0$

| Index | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
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| Actual | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 |
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- $0.48 < T \leq 0.66$: TPR $= 5/7$ and FPR $= 0$
- $0.66 < T \leq 0.86$: TPR $= 4/7$ and FPR $= 0$

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- $0.42 < T \leq 0.43$: TPR $= 5/7$ and FPR $= 2/5$
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- $0.48 < T \leq 0.66$: TPR $= 5/7$ and FPR $= 0$
- $0.66 < T \leq 0.86$: TPR $= 4/7$ and FPR $= 0$
- $0.86 < T \leq 0.90$: TPR $= 3/7$ and FPR $= 0$
- $0.90 < T \leq 0.95$: TPR $= 2/7$ and FPR $= 0$

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| Actual | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 |
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- $0.00 \le T \le 0.05$: TPR $= 1$ and FPR $= 1$
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- $0.66 < T \le 0.86$: TPR $= 4/7$ and FPR $= 0$
- $0.86 < T \le 0.90$: TPR $= 3/7$ and FPR $= 0$
- $0.90 < T \le 0.95$: TPR $= 2/7$ and FPR $= 0$
- $0.95 < T \le 0.98$: TPR $= 1/7$ and FPR $= 0$

| Index | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
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| Actual | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 |
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- $0.00 \leq T \leq 0.05$: TPR = 1 and FPR = 1
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# ROC

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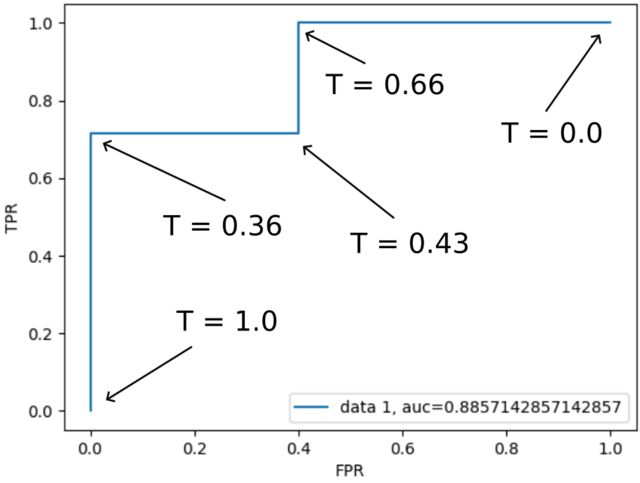
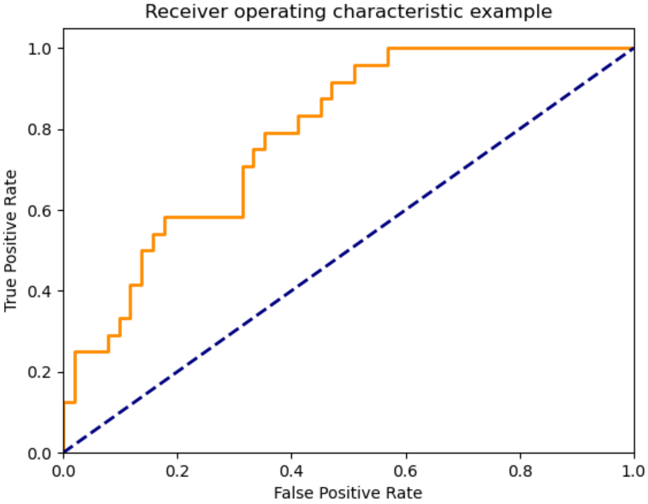
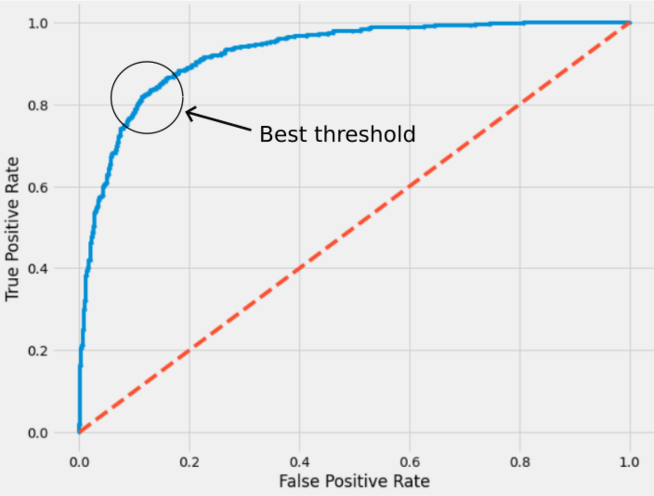


# Iris Dataset - A Classifier



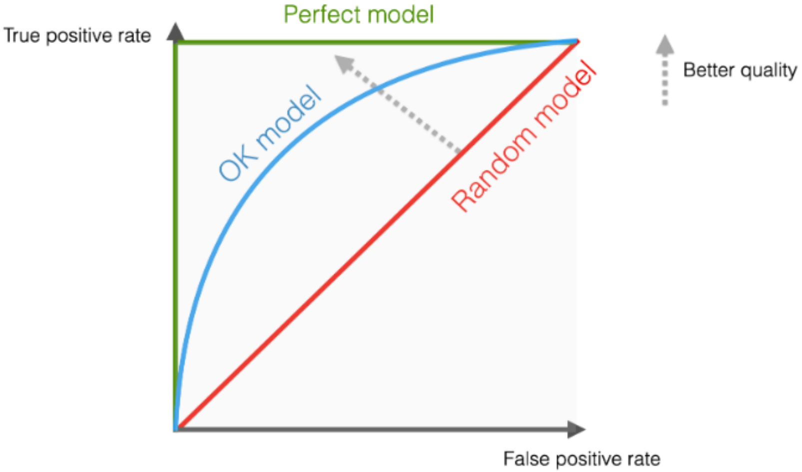

Example from the scikit-learn manual - SVM classifier trained in Iris

# 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. ROC-AUC $\approx 0.5$ indicates random guessing.

# ROC-AUC

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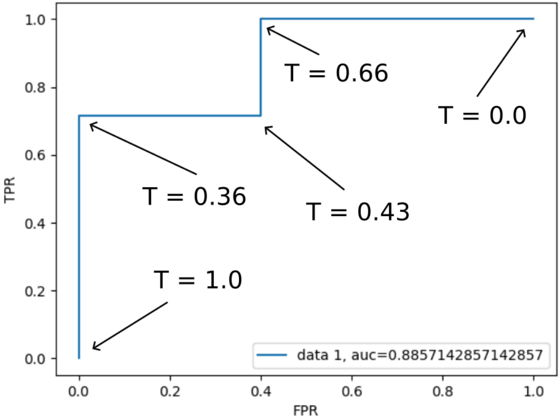
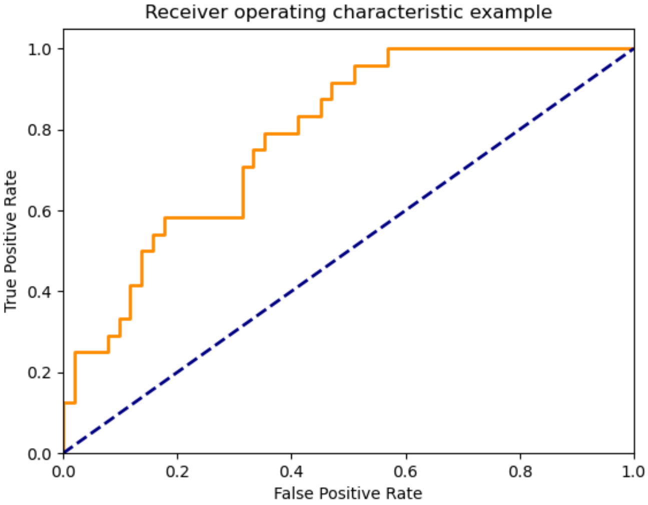



ROC-AUC $= 0.8857$

# 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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- multi-class classifiers,
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- probabilistic classifiers,
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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

In our case, the following scenarios are typical:

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  - Hyperparameter fine-tuning.
  - Comparison of different models (e.g., KNN and decision trees).

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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How to compare $(\text{Precision}_1, \text{Recall}_1)$ of the fist classifier with $(\text{Precision}_2, \text{Recall}_2)$ of the second classifier?

*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

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

- 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** | $8+4=12$ | |

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

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

Consider a threshold $t$ on the Recall.

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

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

# 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.

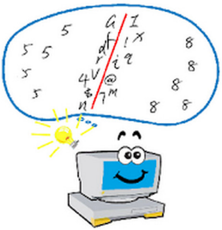
    (Even though this is not the best way of representing images.)

# Basic Problems

We consider two basic problems:

- (Binary) classification

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



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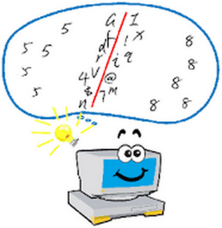

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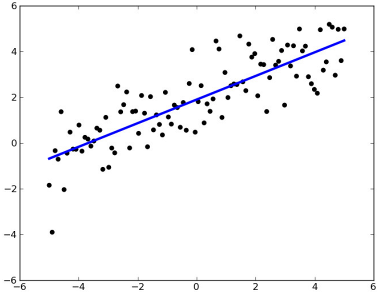


- Regression

  **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:

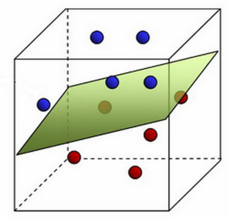
- In practice, we often do not strictly demand $h(\vec{x}) = c$ for all training examples $(\vec{x}, c) \in D$ (often it is impossible)
- We are more interested in good **generalization**, that is how well $h$ classifies new instances that do not belong to $D$.

  (Recall that we usually evaluate accuracy of the resulting hypothesized function $h$ on a test set.)

# Models

We consider two kinds of hypothesis spaces:

- Linear (affine) classifiers (this lecture)



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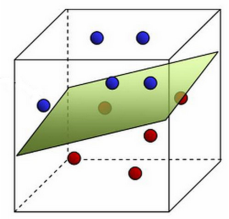
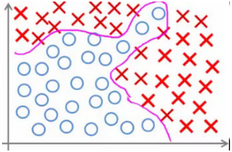
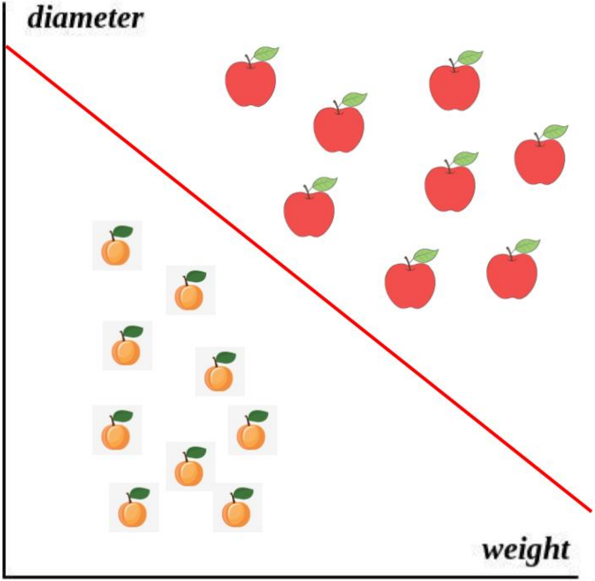


- Non-linear classifiers (kernel SVM, neural networks) (later lectures)



# Linear Classifier – Example



# Length and Scalar Product of Vectors

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- *Scalar product* $\vec{x} \cdot \vec{y}$ of vectors $\vec{x} = (x_1, \ldots, x_n)$ and $\vec{y} = (y_1, \ldots, y_n)$ 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 $\vec{x} \cdot \vec{x} = ||\vec{x}||^2$

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

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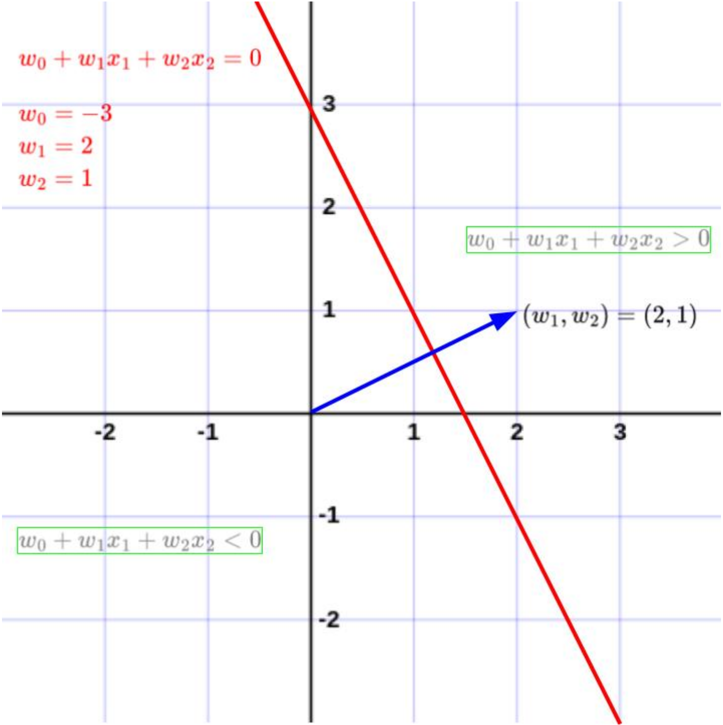
More succinctly:

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

We define separating hyperplane determined by $\vec{w}$ as the set of all $\vec{x} \in \mathbb{R}^n$ satisfying $w_0 + \sum_{i=1}^{n} w_i \cdot x_i = 0$.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2
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-1
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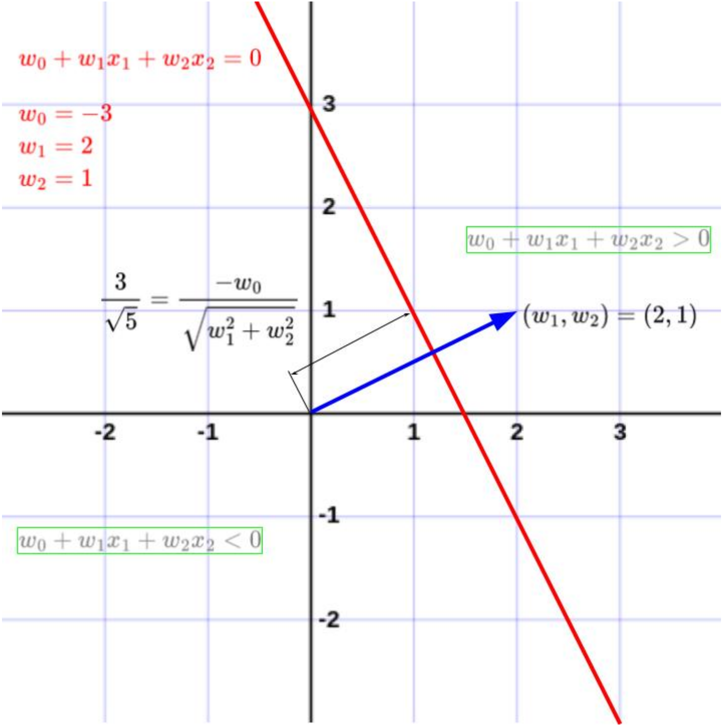
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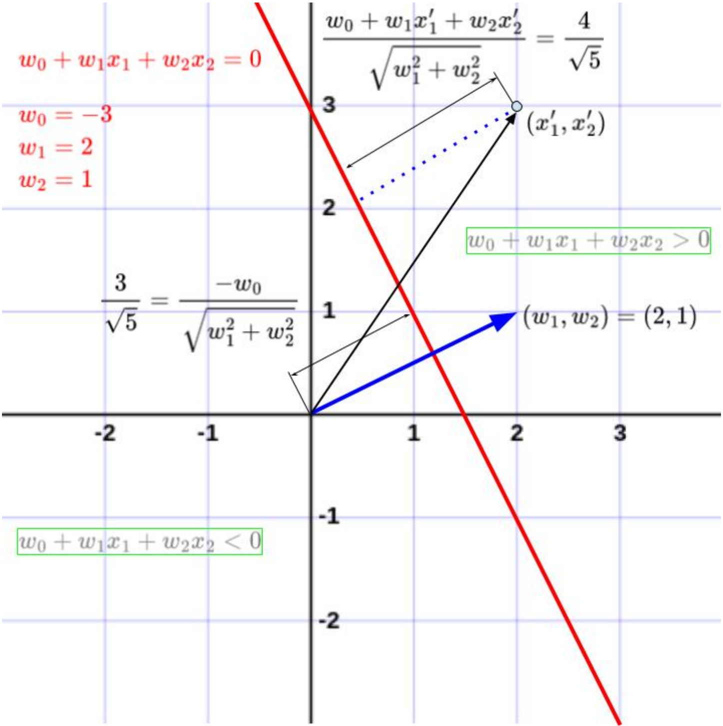
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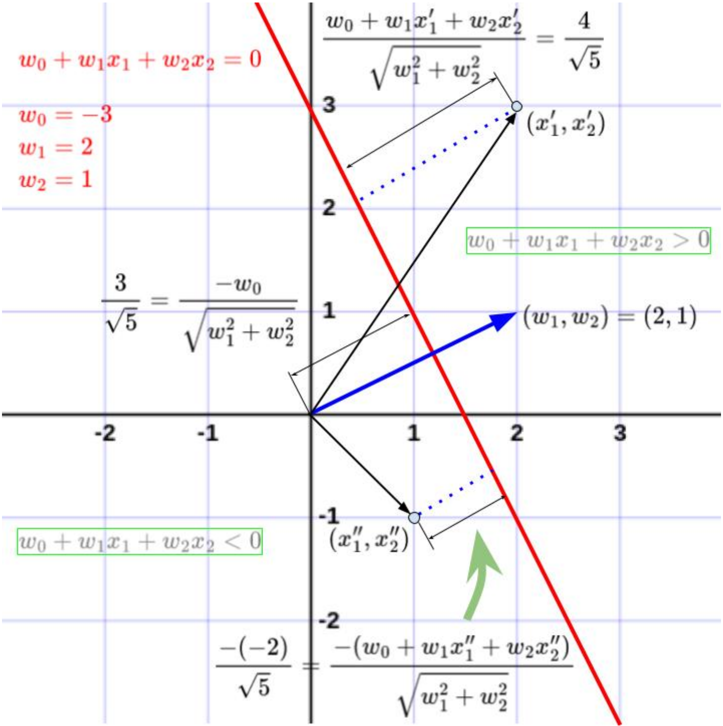
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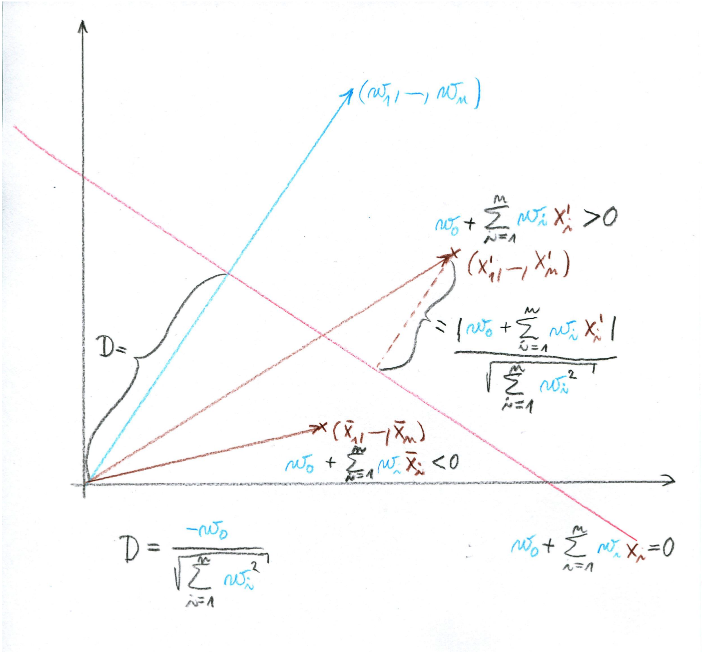
$w_0 + w_1x_1 + w_2x_2 > 0$
$\frac{3}{\sqrt{5}} = \frac{-w_0}{\sqrt{w_1^2 + w_2^2}}$
$(w_1, w_2) = (2, 1)$
$(x_1'', x_2'')$
$w_0 + w_1x_1 + w_2x_2 < 0$
$\frac{-(-2)}{\sqrt{5}} = \frac{-(w_0 + w_1x_1'' + w_2x_2'')}{\sqrt{w_1^2 + w_2^2}}$
-2
-1
1
2
3
3
2
1
-1
-2

# Linear Classifier – Geometry



# Linear Classifier – Notation

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

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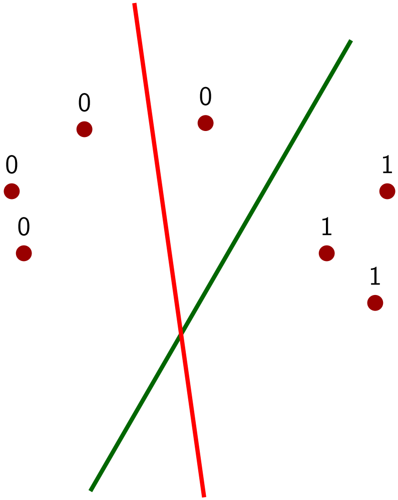
This makes the notation for the linear classifier more succinct:

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

# 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

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

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

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

- A weight vector $\vec{w} \in \mathbb{R}^{n+1}$ is **consistent with** $D$ if

$$h[\vec{w}](\vec{x}_k) = sgn(\vec{w} \cdot \tilde{\mathbf{x}}_k) = c_k \quad \text{for all } k = 1, \ldots, p$$

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- 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 $k = (t \mod p) + 1$, 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:

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

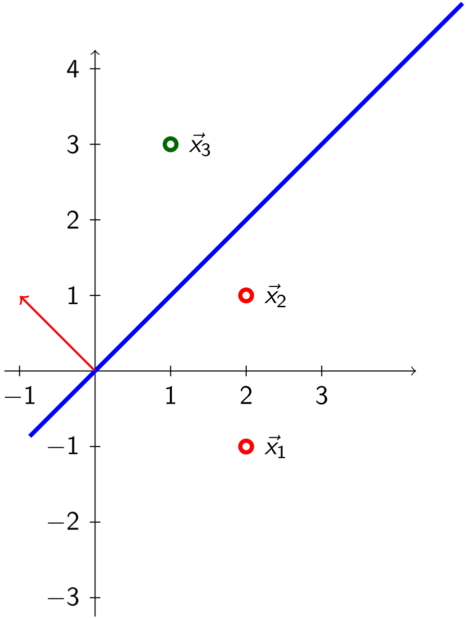
That is

$$\begin{aligned}\vec{x}_1 &= (2,-1) \\ \vec{x}_2 &= (2,1) \\ \vec{x}_3 &= (1,3)\end{aligned} \qquad \begin{aligned}\tilde{\mathbf{x}}_1 &= (1,2,-1) \\ \tilde{\mathbf{x}}_2 &= (1,2,1) \\ \tilde{\mathbf{x}}_3 &= (1,1,3)\end{aligned}$$

$$\begin{aligned}c_1 &= 1 \\ c_2 &= 1 \\ c_3 &= 0\end{aligned}$$

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 $w_0 + w_1 x_1 + w_2 x_2 = 0$.

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

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

and thus

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

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

Hence,

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

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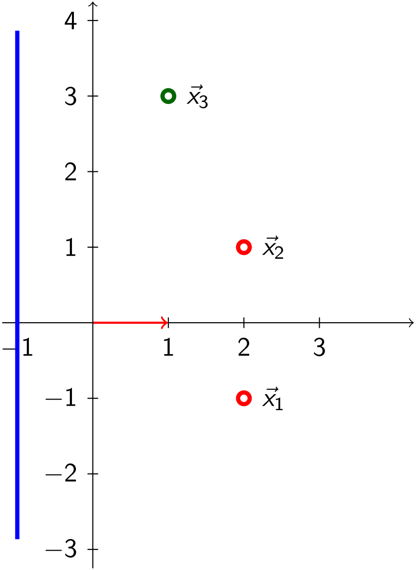


# Example: Computing $\vec{w}^{(2)}$

We have

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

thus

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

and thus

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

(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

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

and thus

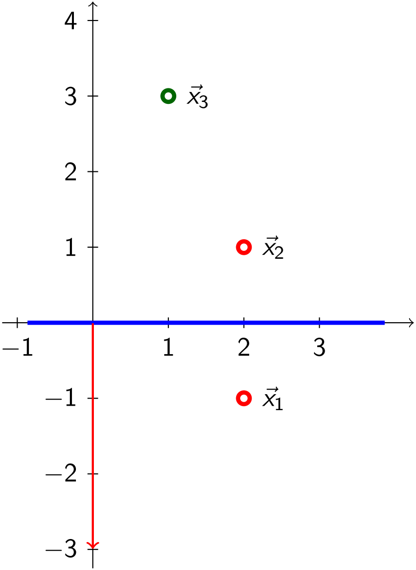
$$sgn\left(\vec{w}^{(2)} \cdot \tilde{\mathbf{x}}_3\right) - c_3 = 1 - 0 = 1$$

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

Hence,

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

# 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

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

and thus

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

(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

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

and thus

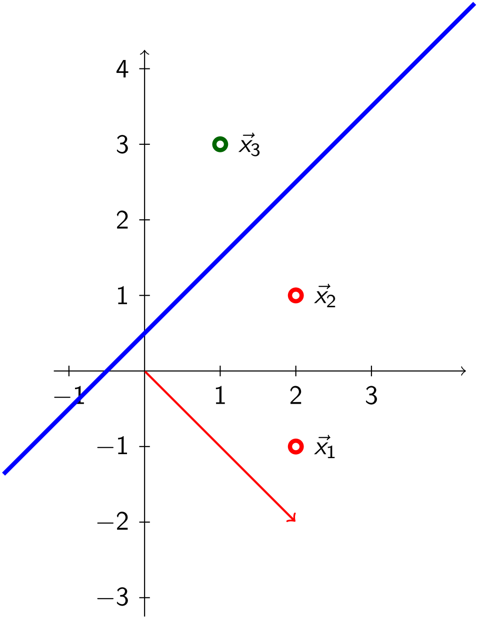
$$sgn\left(\vec{w}^{(4)} \cdot \tilde{\mathbf{x}}_2\right) - c_2 = 0 - 1 = -1$$

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

Hence,

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

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



# Example: The result

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

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

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

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

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

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

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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 |
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| 45 | 9.0 |
| 28 | 6.0 |
| 15 | 1.5 |
| 12 | 1.0 |
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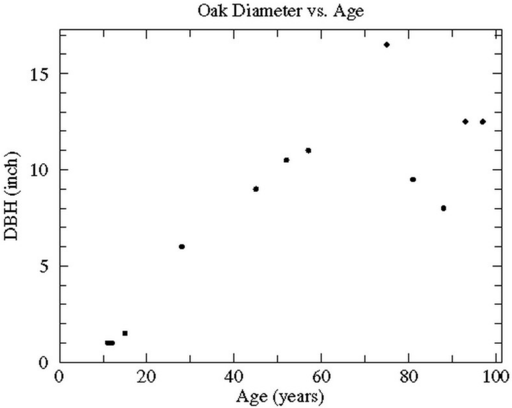

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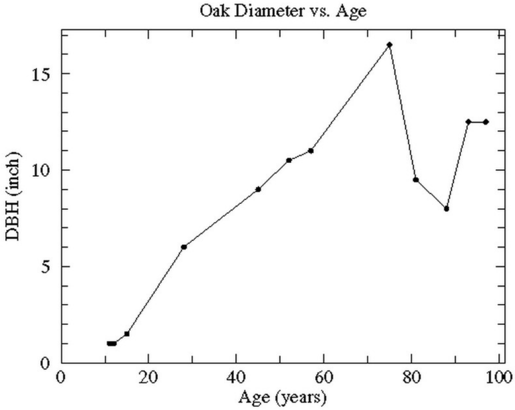


NO!

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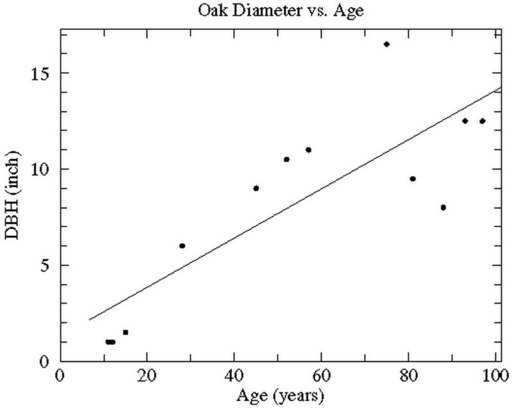


possibly YES!

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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:

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

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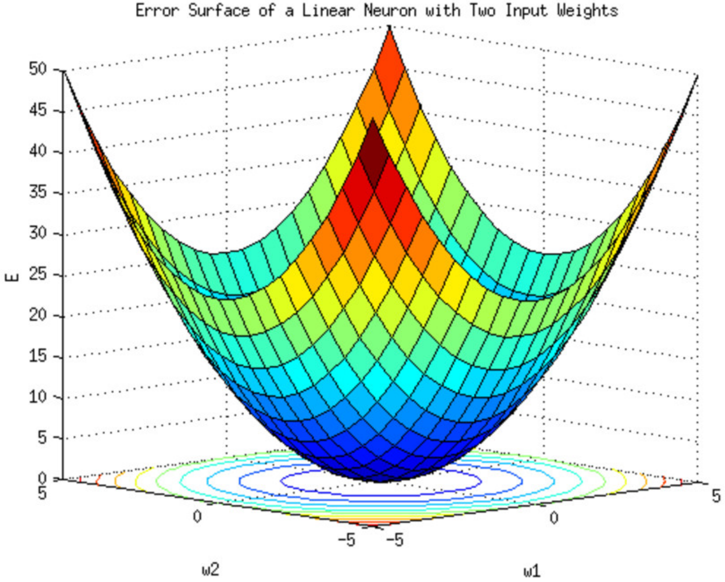
- **Squared Error Function:**

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

# Error function



# Gradient of the Error Function

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

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

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 $E$!

# Gradient of the Error Function

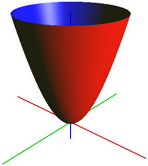
Consider the **gradient** of the error function:

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

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 $E$!

**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.



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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:

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

The augmented feature vectors are: $(1, 2), (1, 3), (1, 4)$.

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$$\nabla E(\vec{w}) = (\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}) =$$
$$(w_0 + w_1 \cdot 2 - 1) \cdot (1, 2) + (w_0 + w_1 \cdot 3 - 2) \cdot (1, 3) + (w_0 + w_1 \cdot 4 - 5) \cdot (1, 4)$$

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## Proposition

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

Training set:

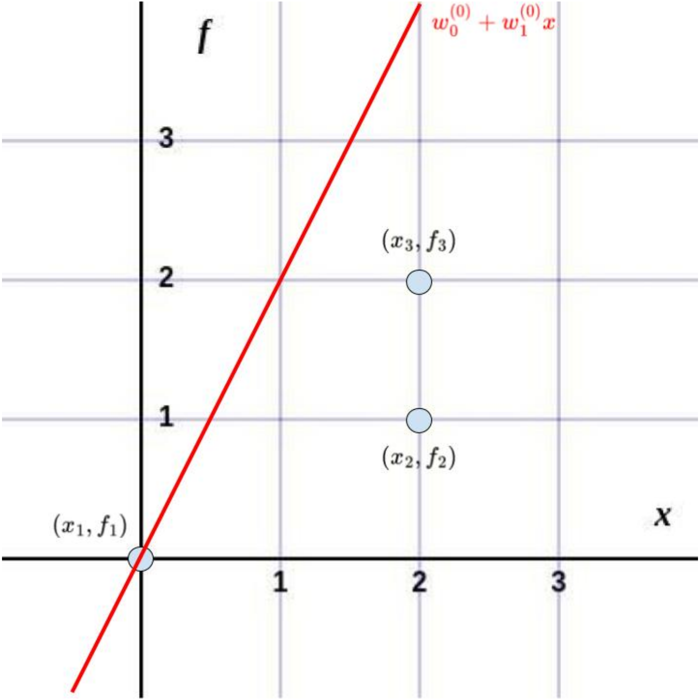
$$D = \{(x_1, f_1), (x_2, f_2), (x_3, f_3)\} = \{(0,0), (2,1), (2,2)\}$$

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

$$\begin{aligned} x_1 &= 0 & \tilde{\mathbf{x}}_1 &= (1, 0) \\ x_2 &= 2 & \tilde{\mathbf{x}}_2 &= (1, 2) \\ x_3 &= 2 & \tilde{\mathbf{x}}_3 &= (1, 2) \end{aligned}$$

$$\begin{aligned} f_1 &= 0 \\ f_2 &= 1 \\ f_3 &= 2 \end{aligned}$$

Assume that the initial vector $\vec{w}^{(0)}$ is $\vec{w}^{(0)} = (w_0^{(0)}, w_1^{(0)}) = (0, 2)$.
Consider $\varepsilon = \frac{1}{10}$.



$w_0^{(0)} + w_1^{(0)}x$
f
3
2
1
$(x_3, f_3)$
$(x_2, f_2)$
$(x_1, f_1)$
x
1
2
3

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

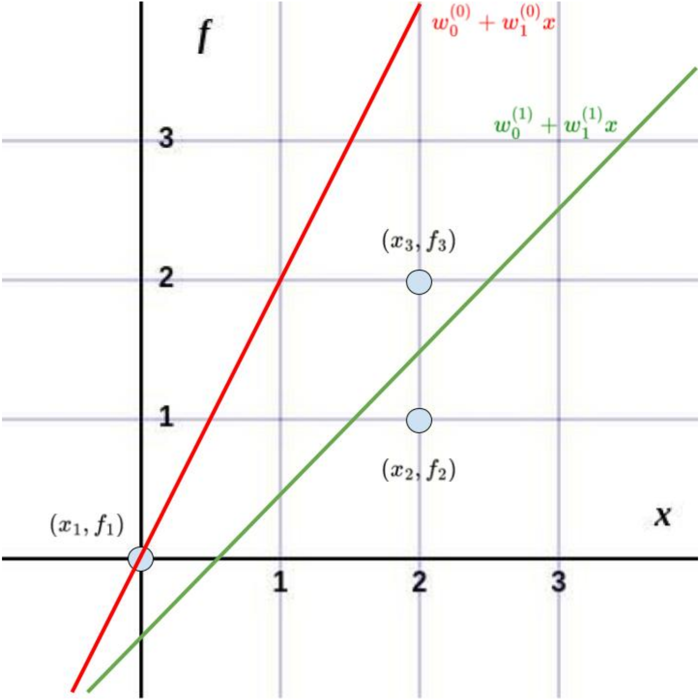
$$\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \frac{\partial E}{\partial w_1}(\vec{w})\right) = (w_0 + w_1 \cdot x_1 - f_1) \cdot \tilde{\mathbf{x}}_1 + (w_0 + w_1 \cdot x_2 - f_2) \cdot \tilde{\mathbf{x}}_2 + (w_0 + w_1 \cdot x_3 - f_3) \cdot \tilde{\mathbf{x}}_3$$

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

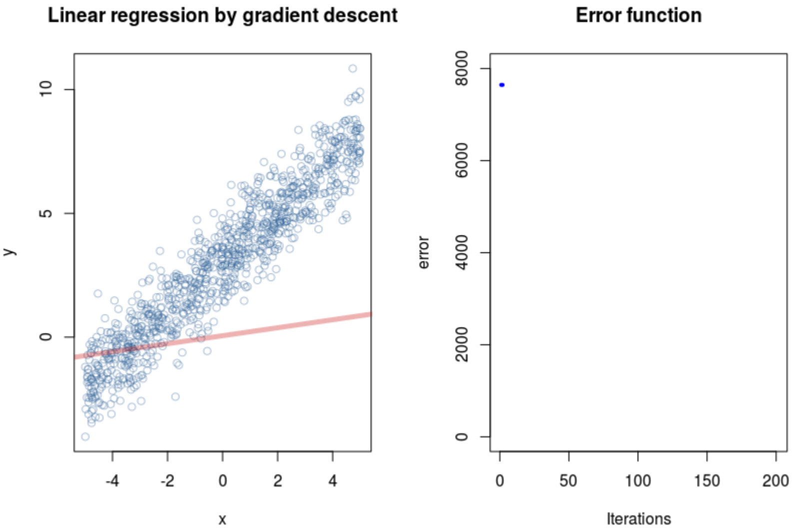
$$\nabla E(\vec{w}^{(0)}) = (0 + 2 \cdot 0 - 0) \cdot (1,0) + (0 + 2 \cdot 2 - 1) \cdot (1,2) + (0 + 2 \cdot 2 - 2) \cdot (1,2) = (3,6) + (2,4) = (5,10)$$

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

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


f
$w_0^{(0)} + w_1^{(0)} x$
$w_0^{(1)} + w_1^{(1)} x$
3
2
1
$(x_3, f_3)$
$(x_2, f_2)$
$(x_1, f_1)$
x
1
2
3

# Linear Regression - Animation



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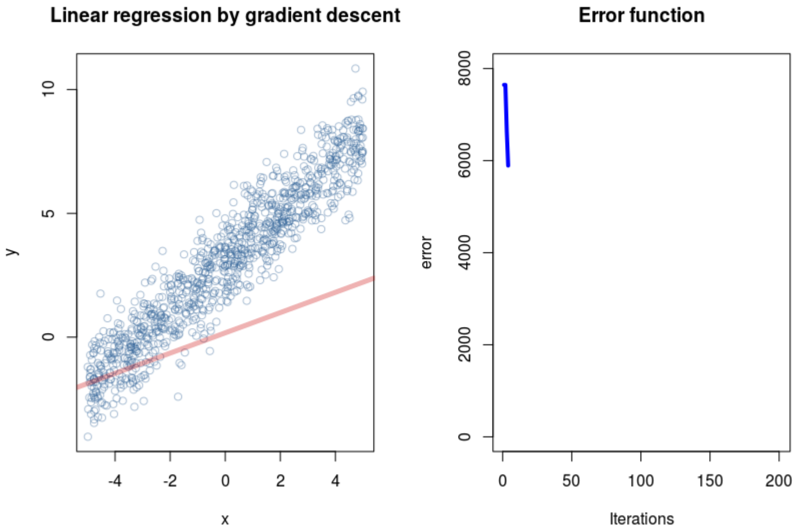

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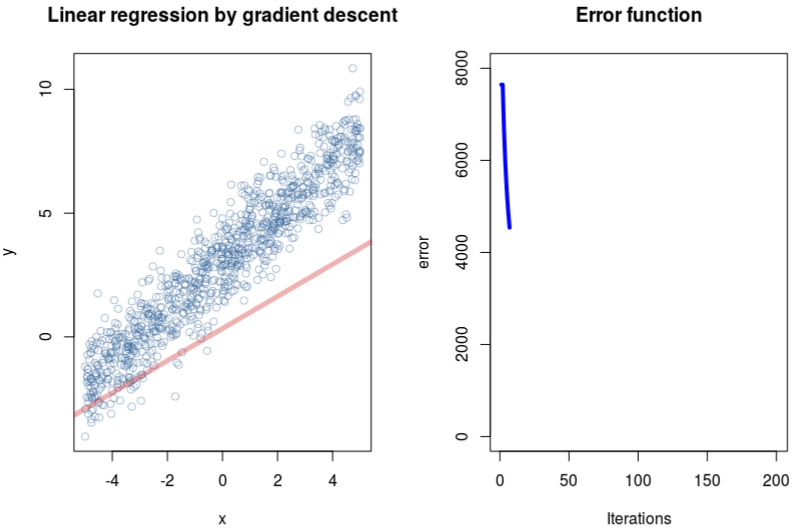

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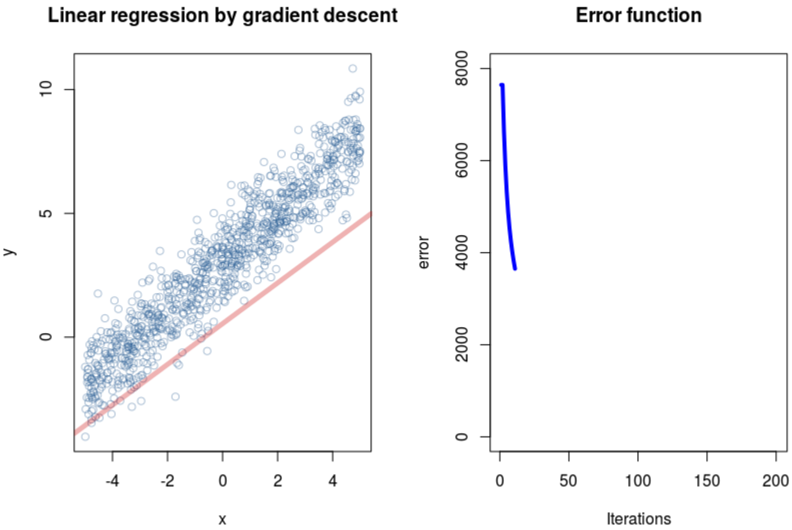

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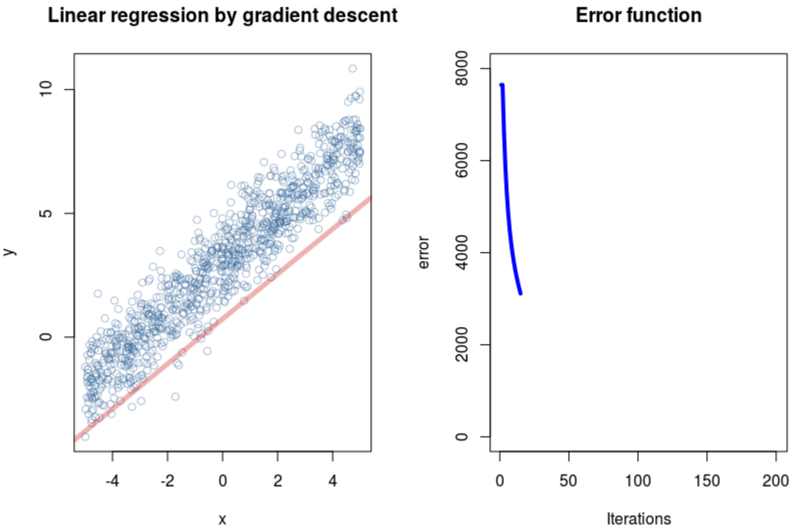

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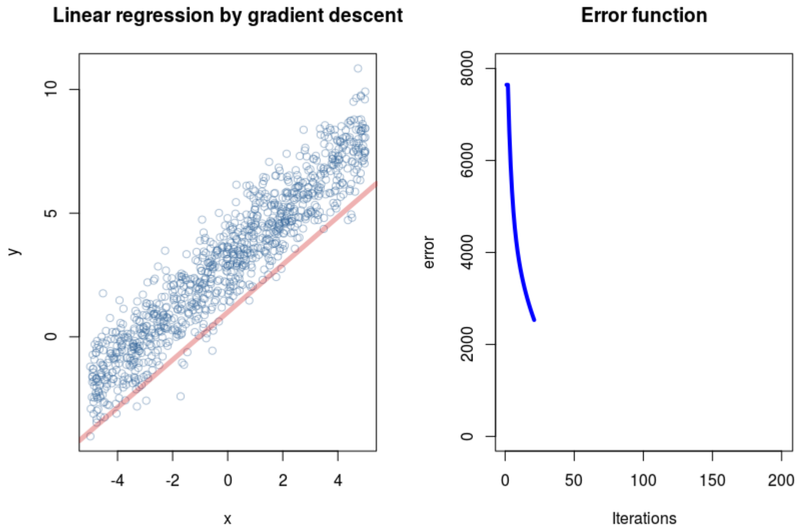

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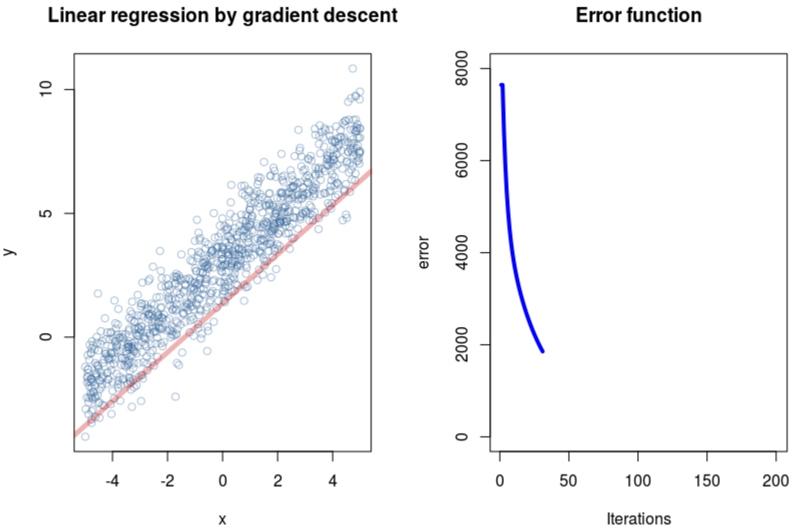

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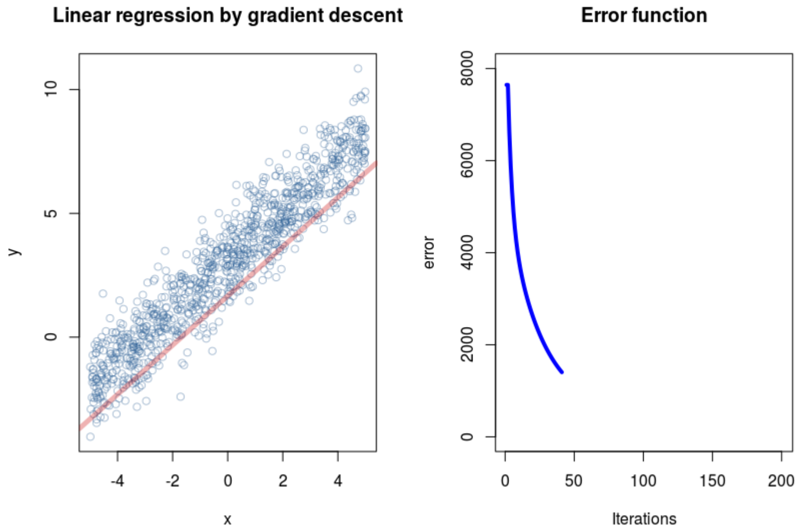

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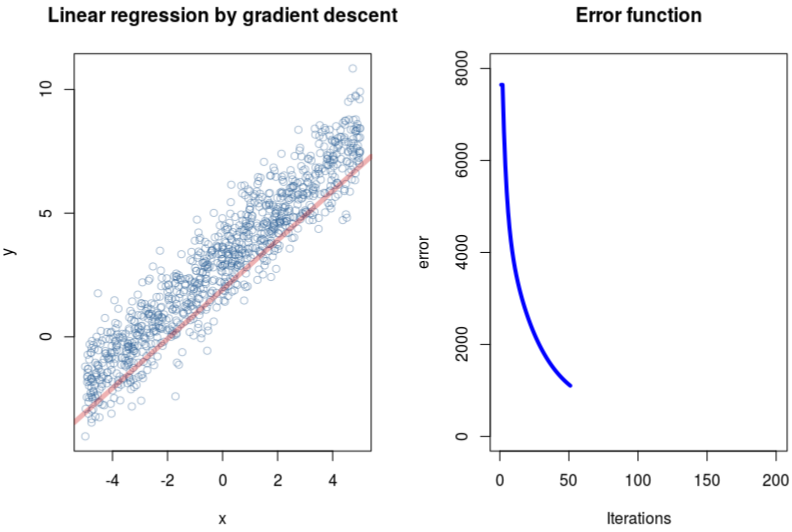

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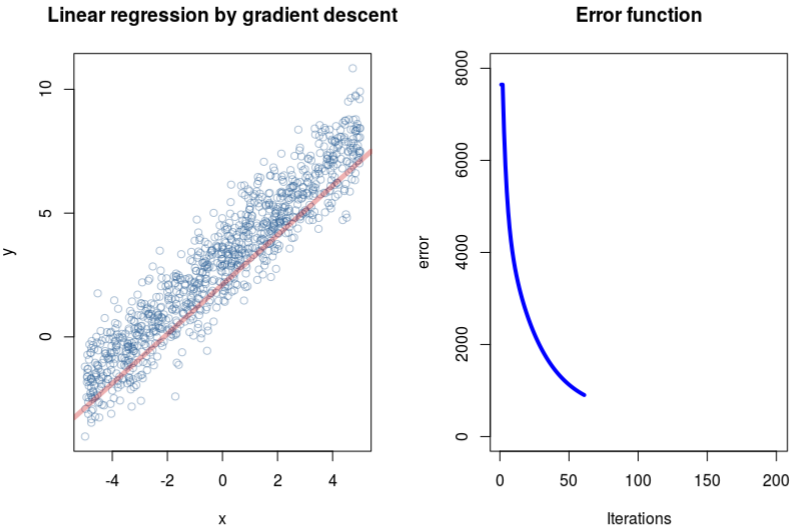

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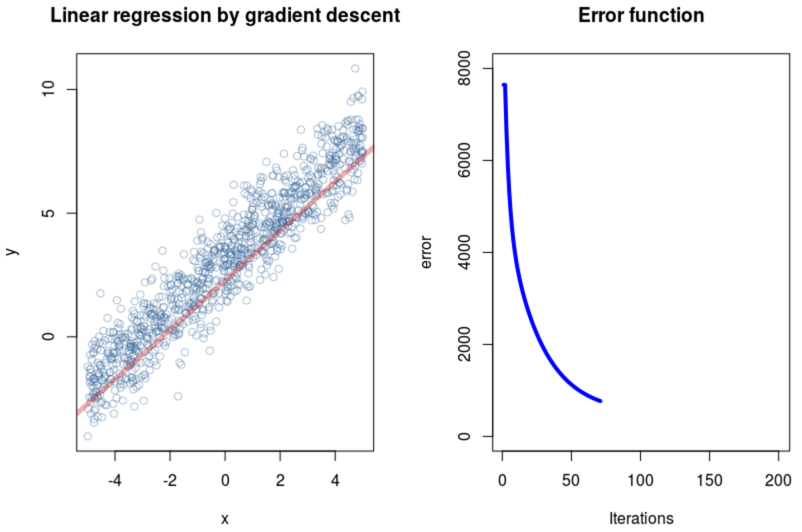

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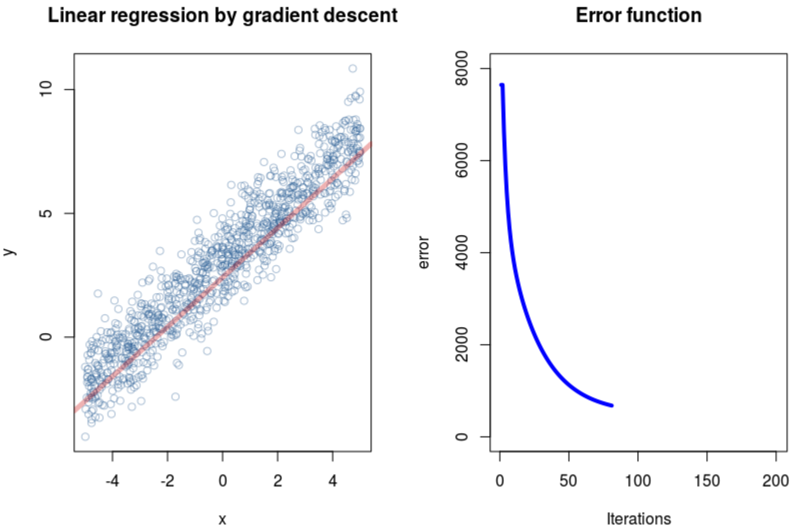

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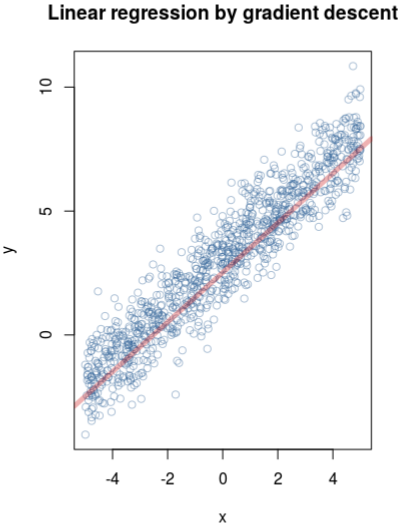


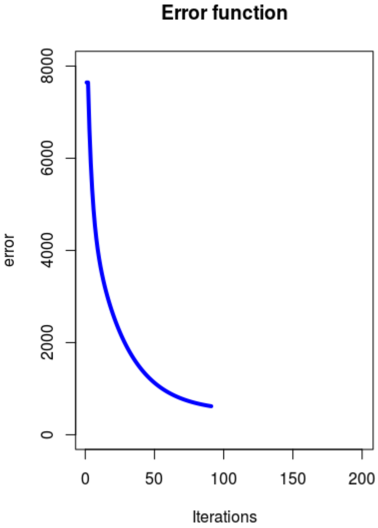

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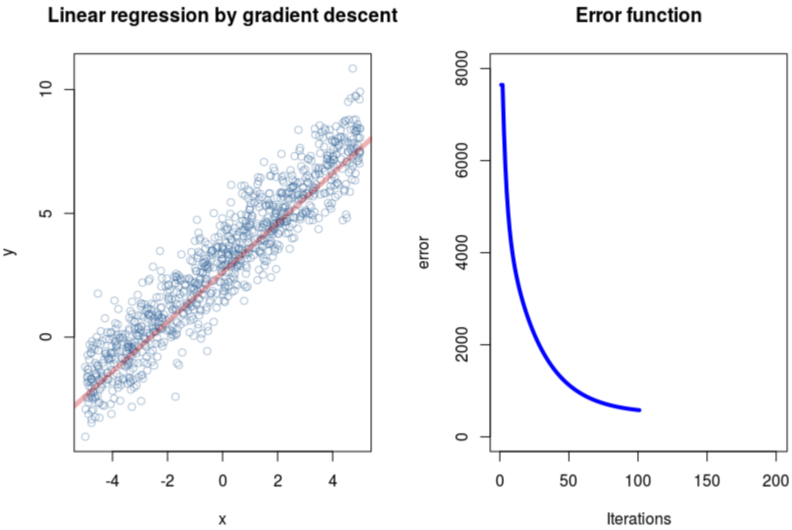

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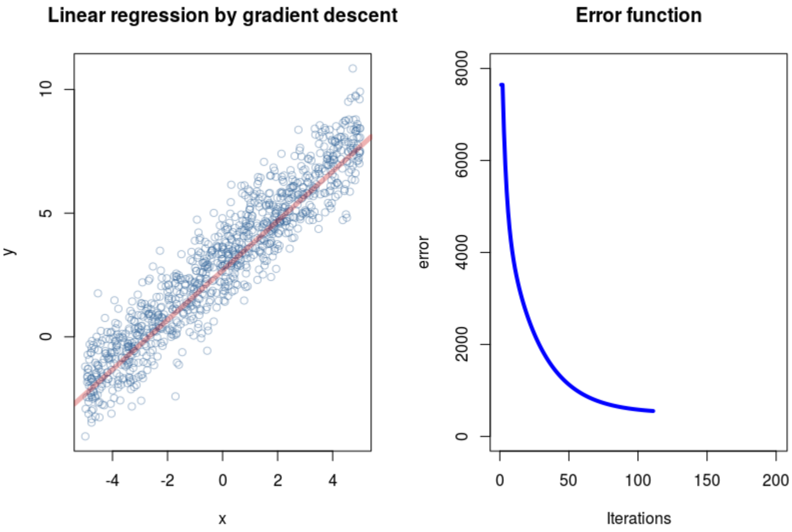

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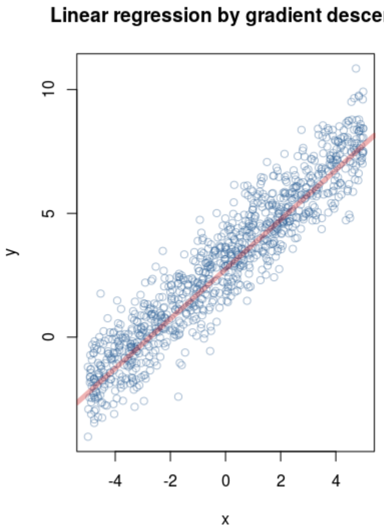


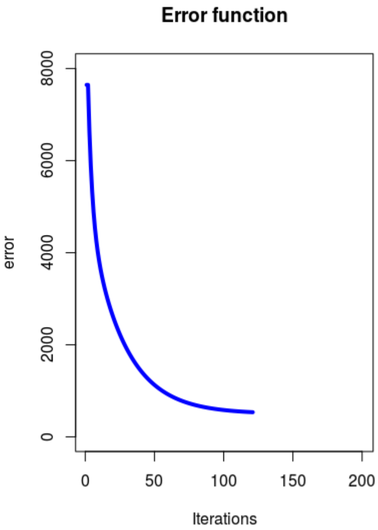

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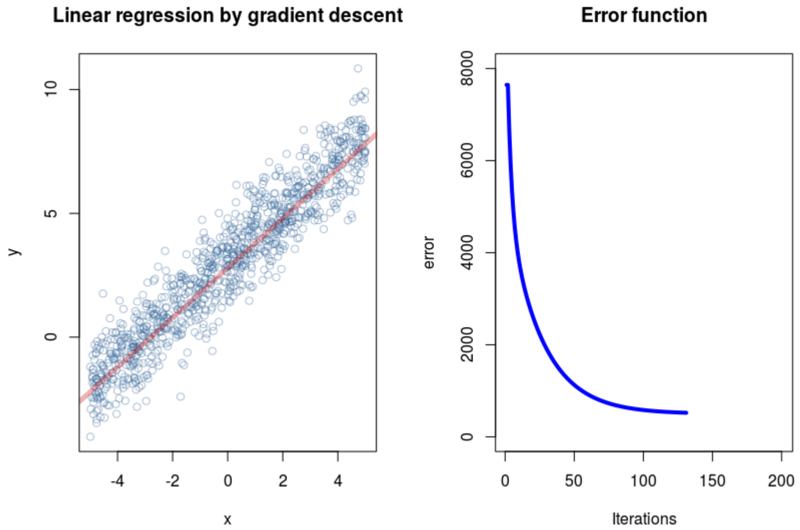

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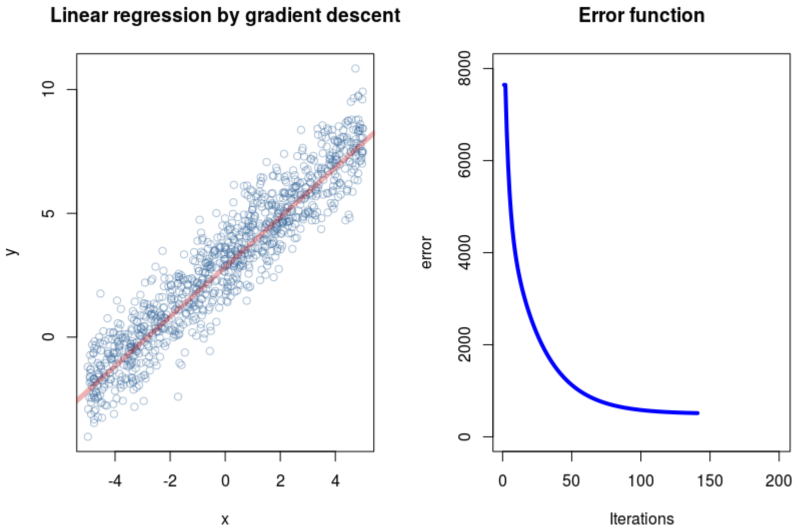

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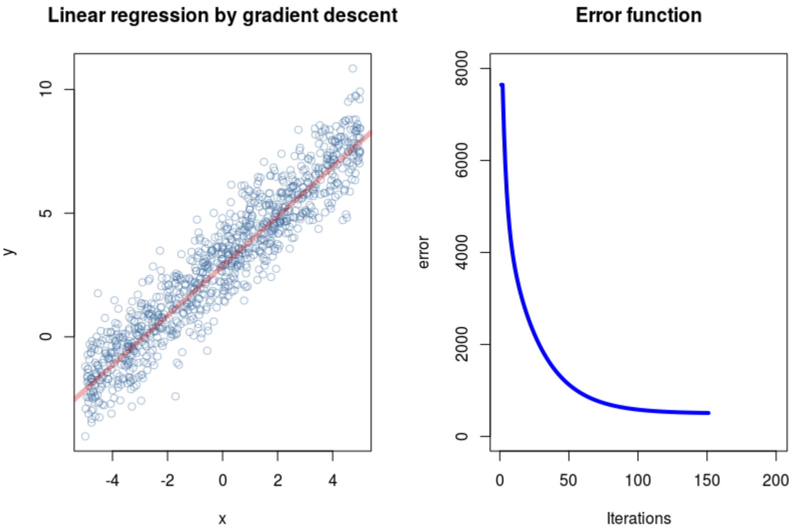

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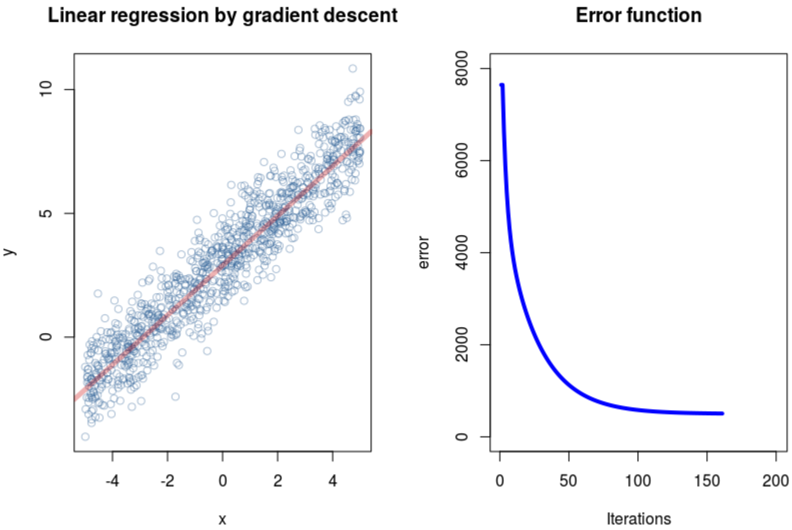

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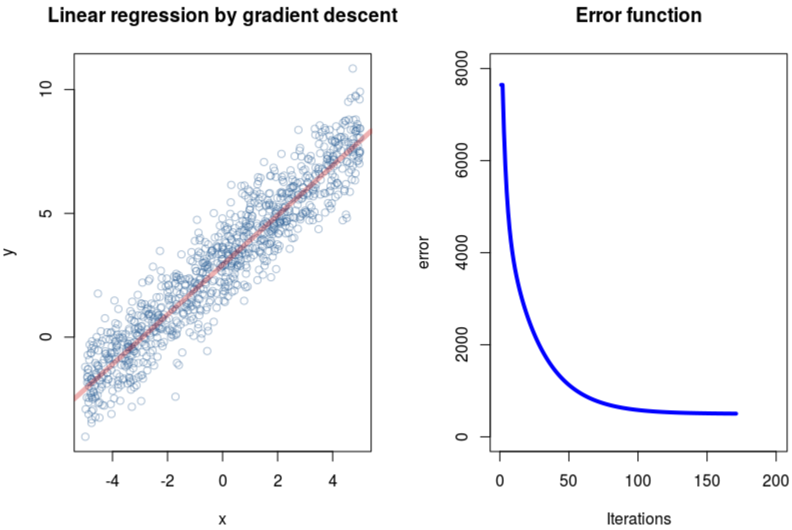

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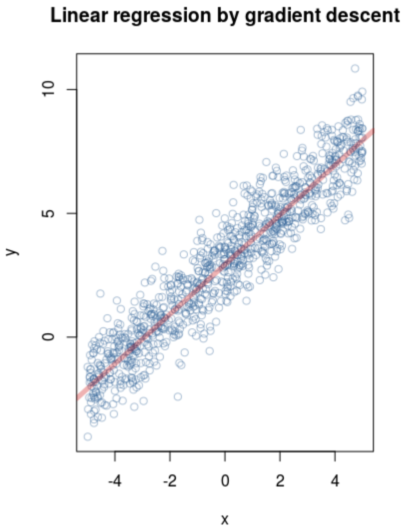


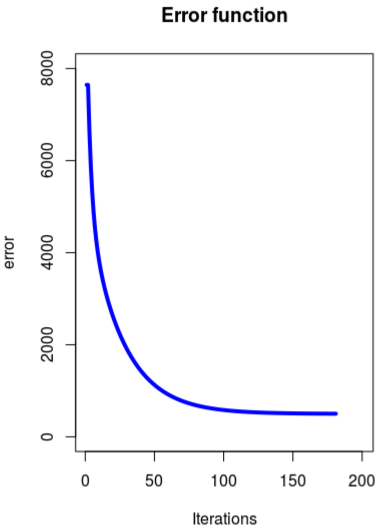

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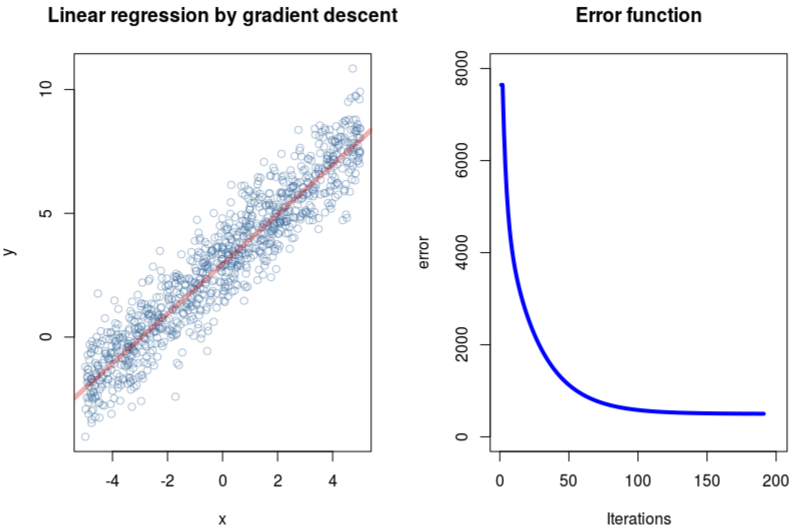

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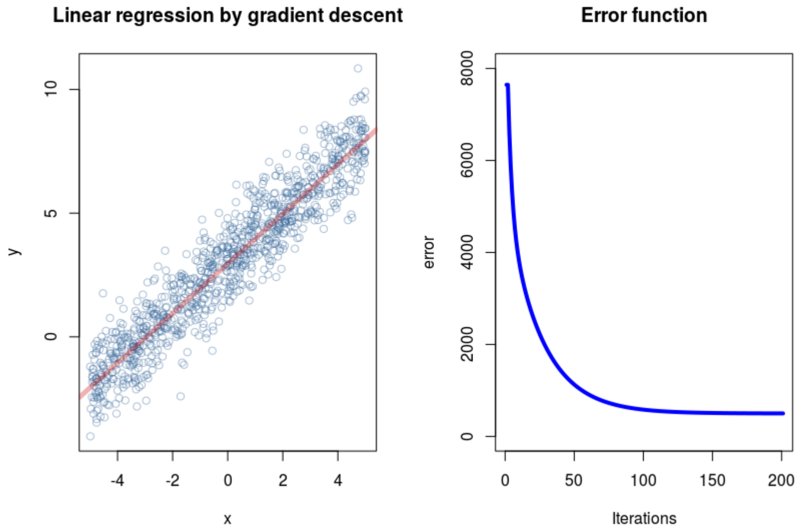

# Finding the Minimum in Dimension One

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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Minimize $E$ w.r.t. $w_0$ a $w_1$:

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

where $\bar{x} = \frac{1}{p} \sum_{k=1}^{p} x_k$ a $\bar{f} = \frac{1}{p} \sum_{k=1}^{p} f_k$

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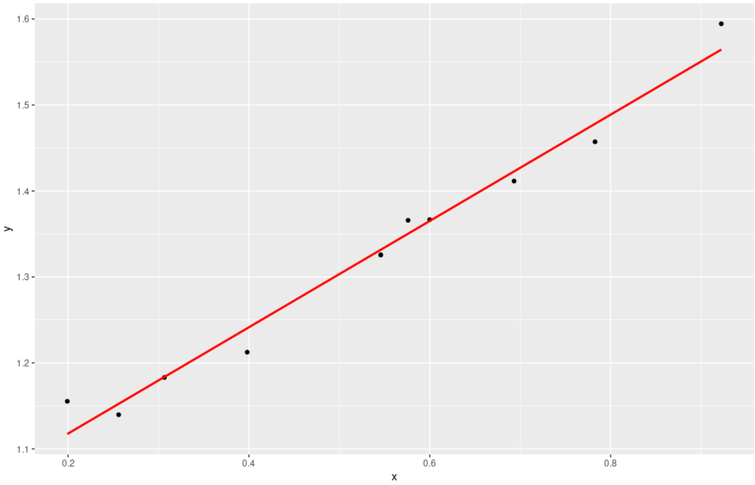
$$\frac{\partial E}{\partial w_1} = 0 \quad \Leftrightarrow \quad w_1 = \frac{\frac{1}{p} \sum_{k=1}^{p} (f_k - \bar{f})(x_k - \bar{x})}{\frac{1}{p} \sum_{k=1}^{p} (x_k - \bar{x})^2}$$

i.e. $w_1 = cov(f, x)/var(x)$

# Effect of Outliers



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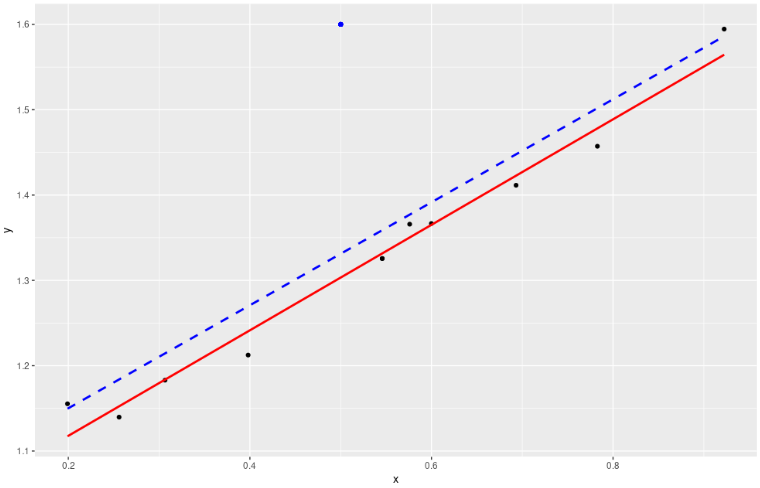

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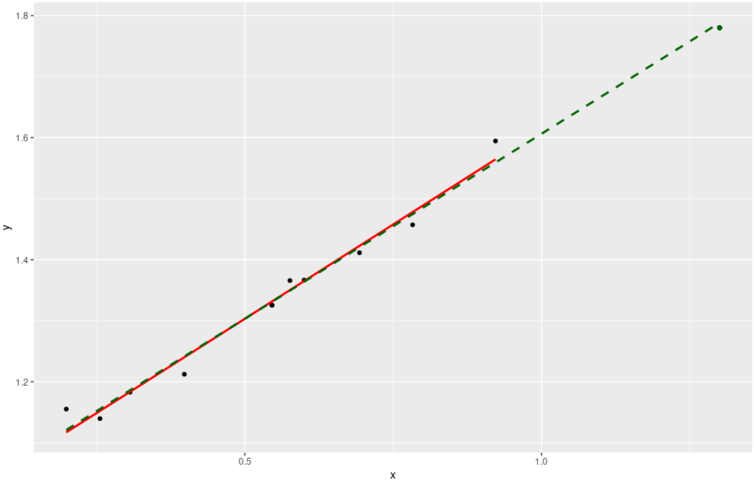

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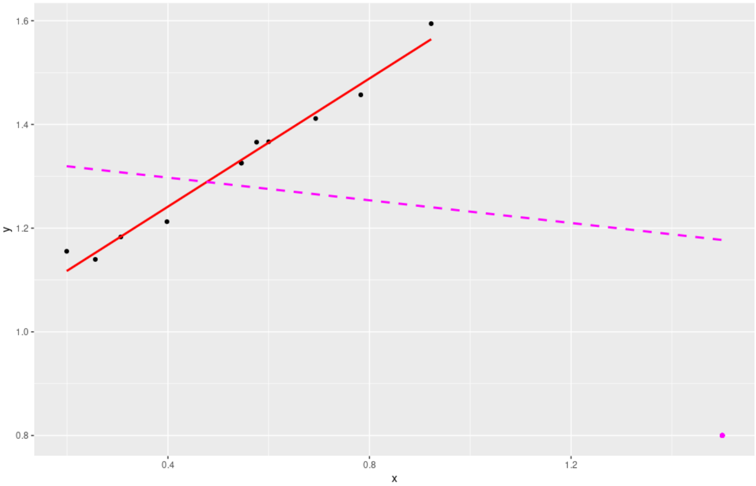

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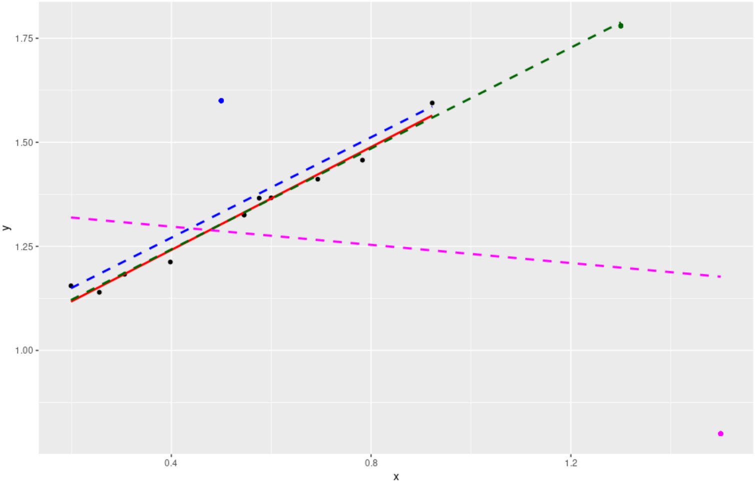
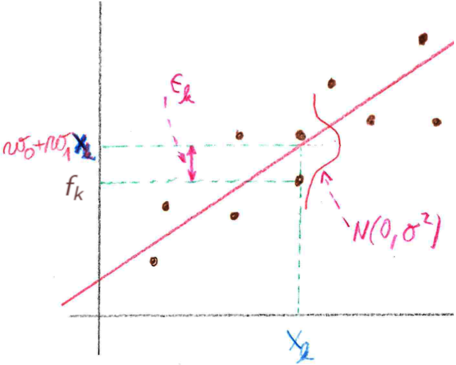


# Maximum Likelihood vs Least Squares (Dim 1)

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

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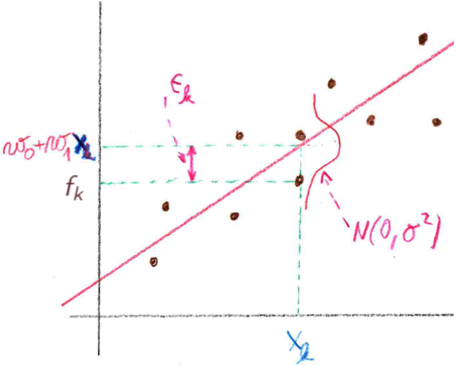


How "probable" is it to generate the correct $f_1, \ldots, f_p$ ?

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 $f_1, \ldots, f_p$ using $f_k = (w_0 + w_1 \cdot x_k) + \epsilon_k$

# Comments on Linear Models

- Linear models are parametric, i.e., they have a fixed form with a small number of parameters that need to be learned from data (as opposed, e.g. to decision trees where the structure is not fixed in advance).

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