IB031 Úvod do strojového učení

Tomáš Brázdil

Course Info

Resources:

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

Evaluation

The evaluation is composed of three parts:

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

Each part contributes the following number of points:

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

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

Distinguishing Properties of the Course

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

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I assume that you have basic knowledge of

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

What Is Machine Learning?

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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 the real price.

Examples (cont.)

In the context of game playing:

- The task T is to play chess.
- The experience E is represented by a series of self-plays where the computer plays against itself.
- The performance measure P is winning/losing the game.
  Here, the trick is to spread the delayed and limited feedback about the result of the game throughout the individual decisions in the game.

Examples (cont.)

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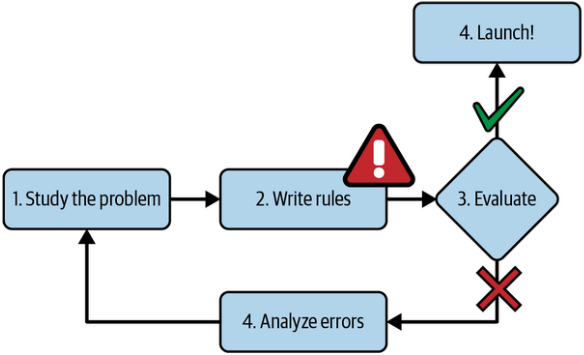
In the context of customer behavior:

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

Comparison of Programming and Learning

How to code the spam filter?

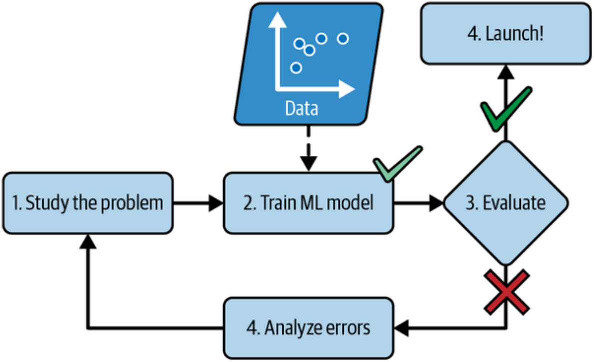
- Examine what spam mails typically contain: Specific words ("Viagra"), sender's address, etc.
- Write down a rule-based system that detects specific features.
- Test the program on new emails and (most probably) go back to look for more spam features.



Comparison of Programming and Learning

The machine learning way:

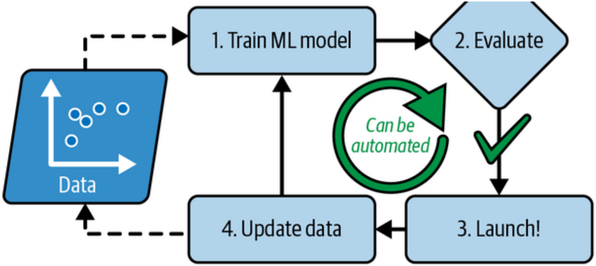
- Study the problem and collect lots of emails, labeling them spam or ham.
- Train a machine learning model that reads an email and decides whether it's spam or ham.
- Test the model and (most probably) go back to collect more data and adjust the model.



ML Solutions are Adaptive

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

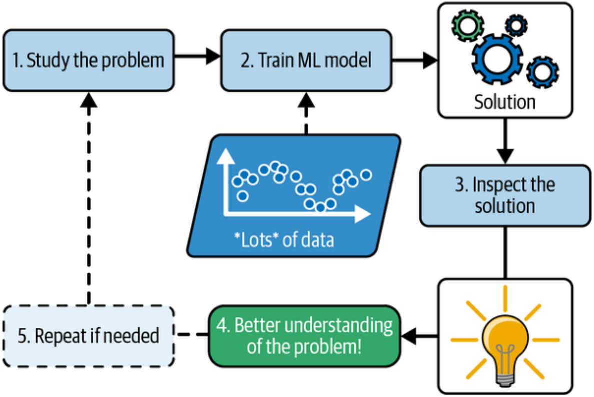
ML systems can be adjusted to new situations by retraining on new data (unless the data becomes ugly).



ML for Human Understanding

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

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



Usage of Machine Learning

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

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

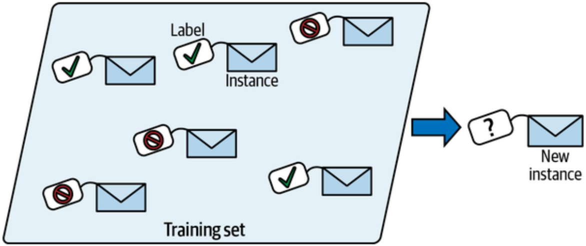
In summary, machine learning offers innovative solutions and adaptability for today's complex and ever-changing problems, (sometimes) providing insights beyond the reach of traditional approaches.

Types of Learning

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

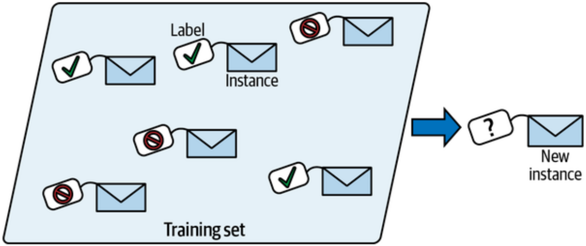
- Supervised learning
- Unsupervised learning
- Semi-supervised learning
- Self-supervised learning
- Reinforcement learning

Supervised Learning



Labels are available for all input data.

Supervised Learning



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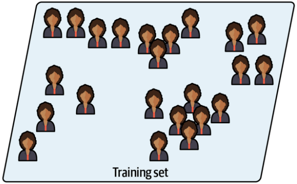
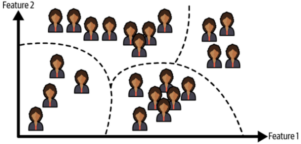
Typical supervised learning tasks are

- *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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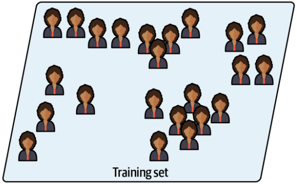

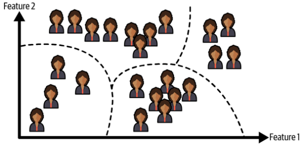

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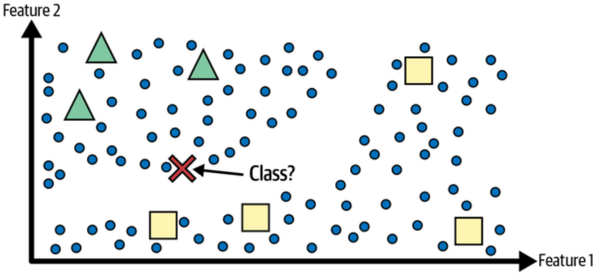
Typical unsupervised learning tasks are

- *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.

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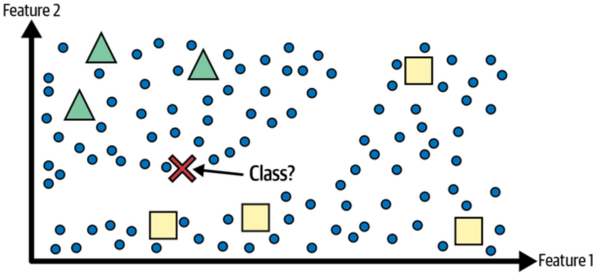
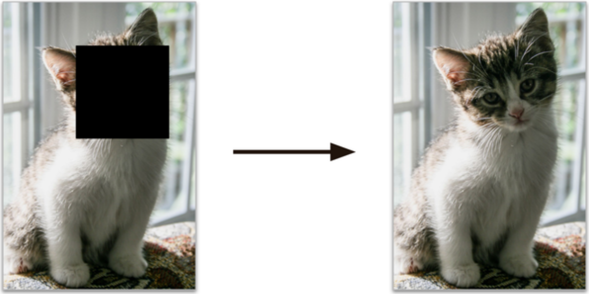


Labels for some data.

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

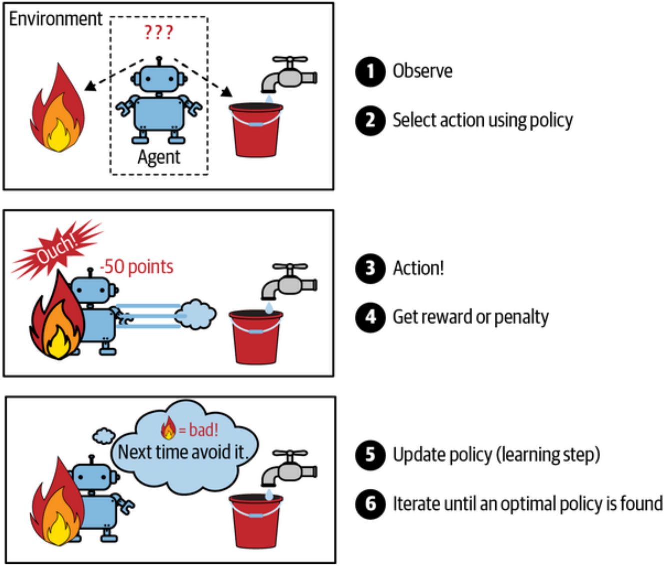


Generate labels from (unlabeled) inputs.

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

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  - The basis forms a generative language model, i.e., a text-generating model trained on texts in a self-supervised way
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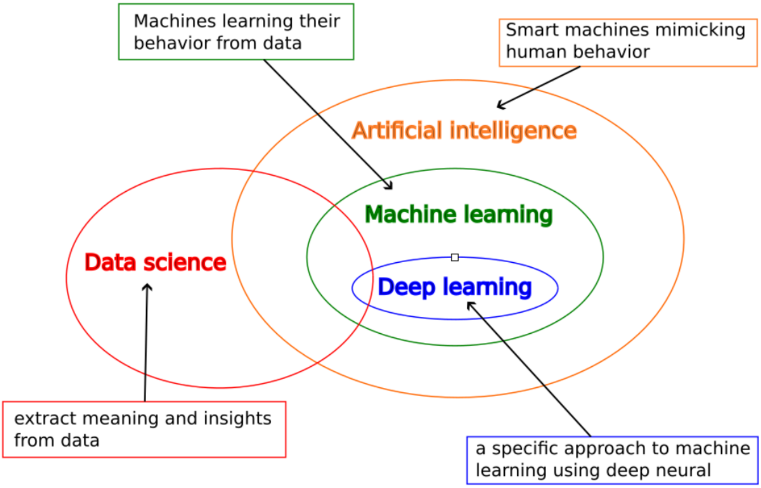
- Game playing: More fancy than useful, learning models beating humans in several difficult games.

ML in Context



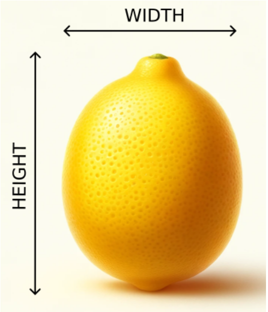
Supervised Learning

Example - Fruit Recognition

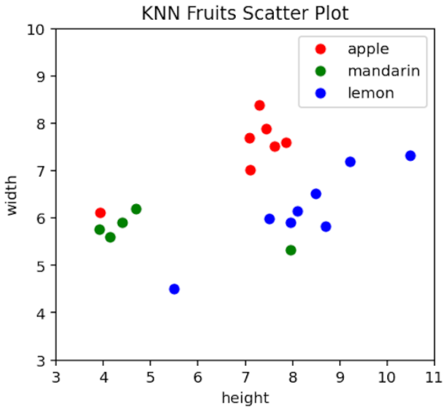
The goal: Create an automatic system for fruit recognition, concretely apple, lemon, and mandarin.

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



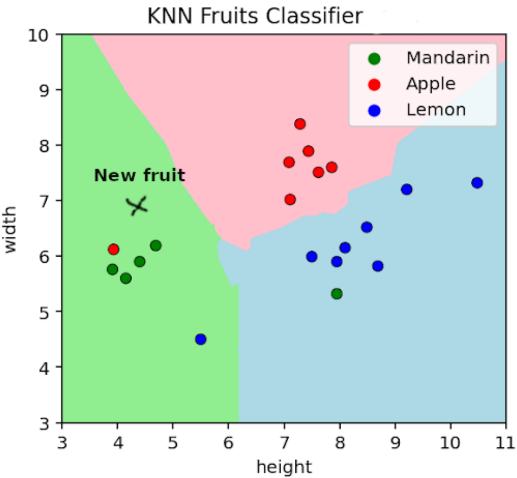
Use similarity to solve the problem.

	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

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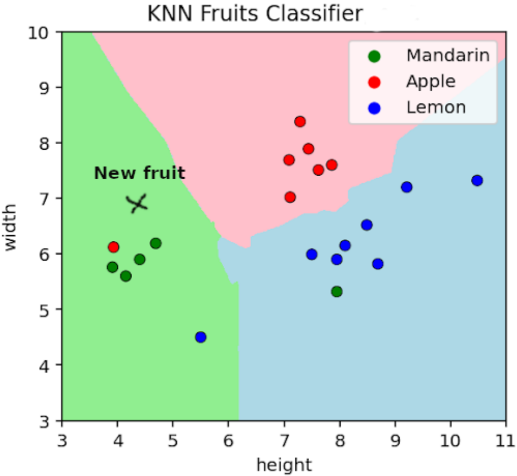
Among the five closest:

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



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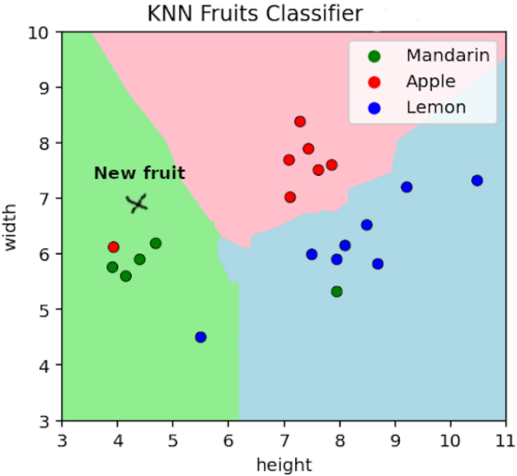
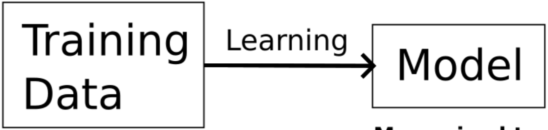
It is a **mandarin**!



Where is the machine learning?

Learning in Fruit Classification with KNN

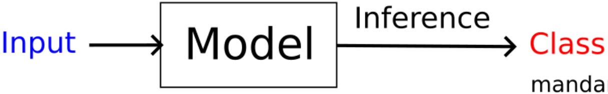
Learning:



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*

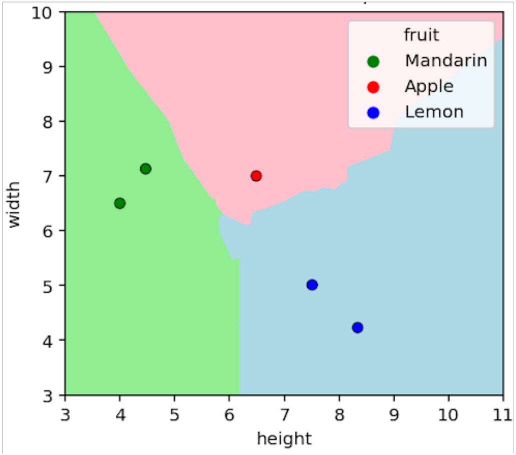
Find K examples $\{E_1, \ldots, E_K\}$ in the dataset whose dimensions are closest to the dimensions of the fruit F
Count the number of examples of each class in $\{E_1, \ldots, E_K\}$
  M mandarins in $\{E_1, \ldots, E_K\}$
  L lemons in $\{E_1, \ldots, E_K\}$
  A apples in $\{E_1, \ldots, E_K\}$
if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

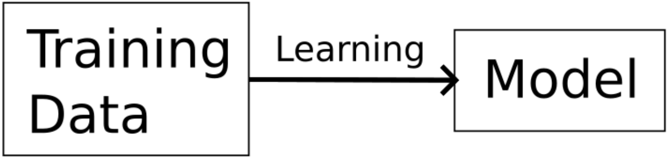
K Nearest Neighbors

…on ideal data

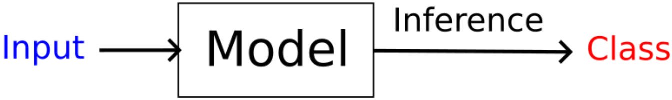
Learning and Inference

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.

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

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

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

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

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

2: For every $c \in C$ count the number $\#c$ of elements ℓ 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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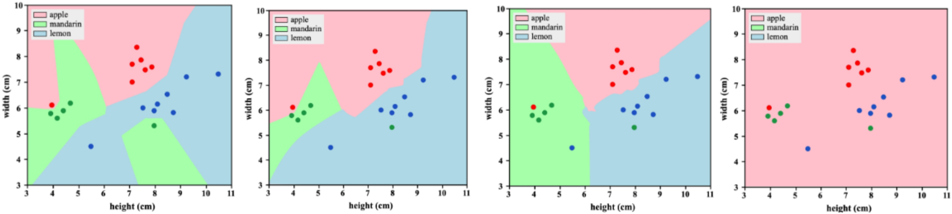
Note that different settings of K lead to different classifiers (for the same d):



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- Deal with issues in the data
  - Data almost always comes in weird formats, with inconsistencies, missing values, wrong values, etc.
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- 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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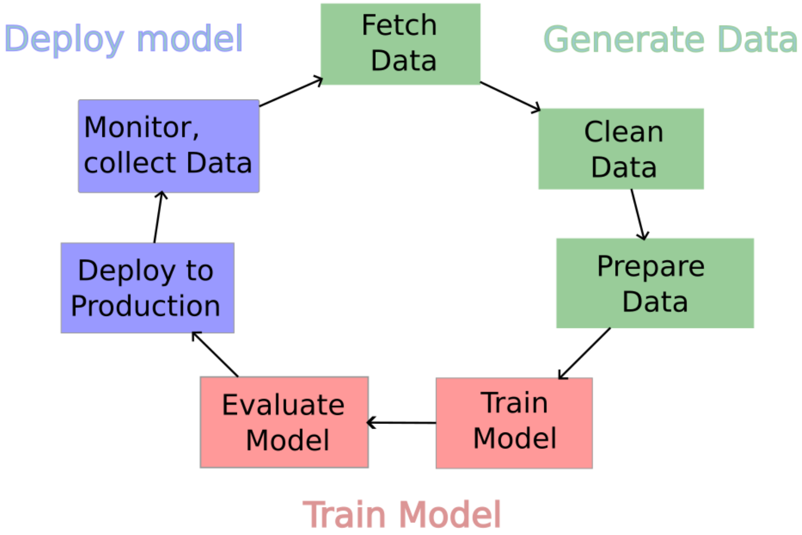
. . . but first, let us see the whole machine-learning pipeline.

Machine Learning Pipeline



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- Collect the data.
  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 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 $m << n$.

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

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

Train Model

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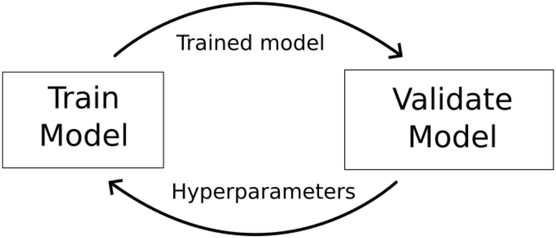
Before training, we should split the dataset into

- *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.

For example, new expensive and difficult measurements are needed 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.

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Data Science Example

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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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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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Researcher: Yes, fields 2 and 3 are basically the same, but I assume that you probably noticed that.
Data Miner: Yes, but these fields were only weak predictors of field 5.

Model Discussion

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.

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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.
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- **Examples:**

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

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

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Binary attributes are categorical attributes with only two values.

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

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Categorical and ordinal attributes are called *qualitative* attributes.

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

Data Types - Numeric Attributes

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

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

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- *Continuous*

  A continuous range of values, an interval.

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

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

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

Decision Trees

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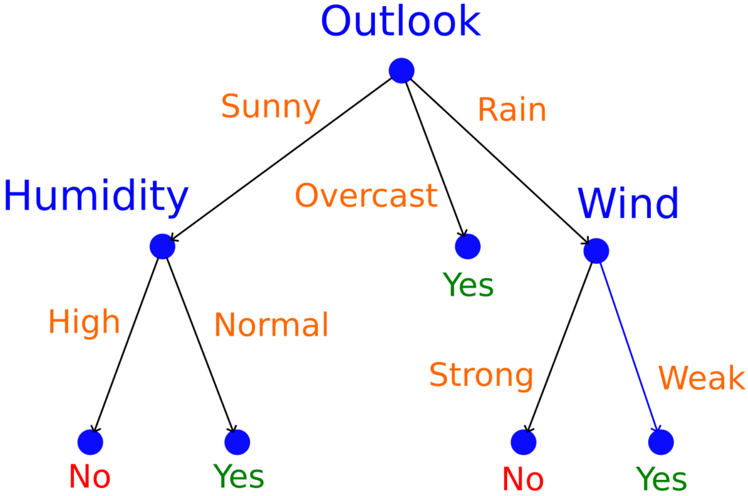
- We will consider the ID3 algorithm.
  Quinlan, 1979
- Various adjustments that appear in C4.5, CART, etc.

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



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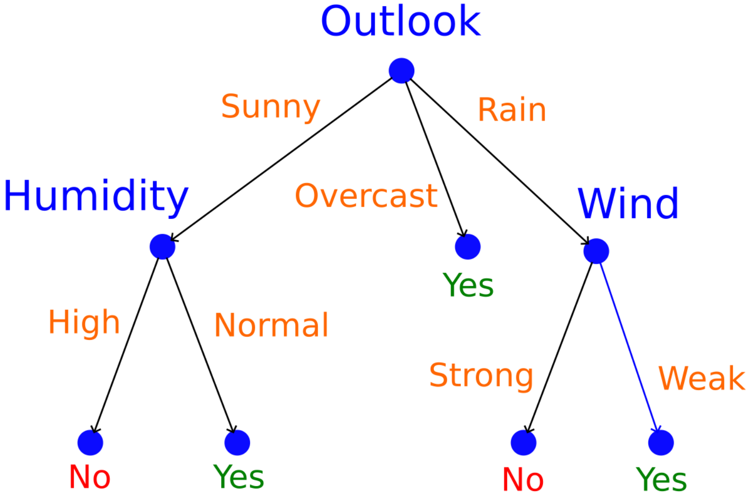

How do we obtain such a tree based on experience/data?

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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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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  - $V(A_3) = \{\mathit{High}, \mathit{Normal}\}$
  - $V(A_4) = \{\mathit{Strong}, \mathit{Weak}\}$
- Consider

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

Example

The tennis problem:

- The attributes are:

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

- The sets of values of the attributes:
  - $V(A_1) = \{\textit{Sunny}, \textit{Overcast}, \textit{Rain}\}$
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  $$\vec{x} = (\textit{Overcast}, \textit{Hot}, \textit{Normal}, \textit{Weak}) \in V(A_1) \times V(A_2) \times V(A_3) \times V(A_4)$$

  Then

  $$A_3(\vec{x}) = \textit{Humidity}(\vec{x}) = \textit{Normal}$$

  $$A_4(\vec{x}) = \textit{Wind}(\vec{x}) = \textit{Weak}$$

Example

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- The attributes are:

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  - $V(A_2) = \{Hot, Mild, Cool\}$
  - $V(A_3) = \{High, Normal\}$
  - $V(A_4) = \{Strong, Weak\}$
- Consider

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  $$A_3(\vec{x}) = Humidity(\vec{x}) = Normal$$

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

Decision Trees

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 $C(\tau) \in C$,
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- and there is a bijection between edges from τ and values of the attribute $A(\tau)$. Given an edge $(\tau, \tau') \in E$ we write $V(\tau, \tau')$ to denote the value of the attribute $A(\tau)$ assigned to the edge.

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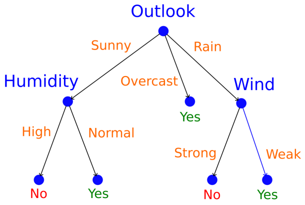
Inference: Given an input $\vec{x}$, we traverse the tree from the root to a leaf, always choosing edges labeled with values of attributes from $\vec{x}$. The output is the class labeling the leaf.

Example

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

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



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

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

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

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

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

Training Dataset

Consider a *training dataset*

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

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

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

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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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  - create a root node τ of a decision tree,
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  - for every $v \in V(A)$ introduce an edge (τ, τ_v) assigned v.

function $\mathrm{ID3}$(dataset $\mathcal{D}$, attribute set $\mathcal{A}$)
Create a root node τ for the tree
if $\mathcal{D} = \emptyset$ **then**
Return the single node τ 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 τ is assigned c
else if set of attributes $\mathcal{A}$ is empty **then**
Return the single-node tree where τ 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 τ to A
for each value $v \in D(A)$ **do**
Compute a decision tree ID3($\mathcal{D}_v, \mathcal{A} \setminus \{A\}$) with root τ_v,
add a new edge (τ, τ_v) assigned v.
end for
end if
return τ
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

The information gain is based on the notion of entropy.

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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

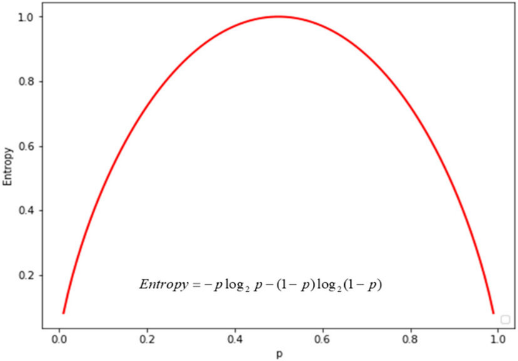
$$Gain(\mathcal{D}, A) = Entropy(\mathcal{D}) - \sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Entropy(\mathcal{D}_v)$$

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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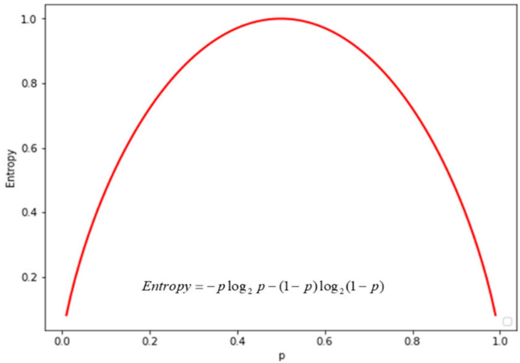

- $\sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Entropy(\mathcal{D}_v)$ is weighted uncertainty of classes in each $\mathcal{D}_v$ (weighted by the relative size of $\mathcal{D}_v$).

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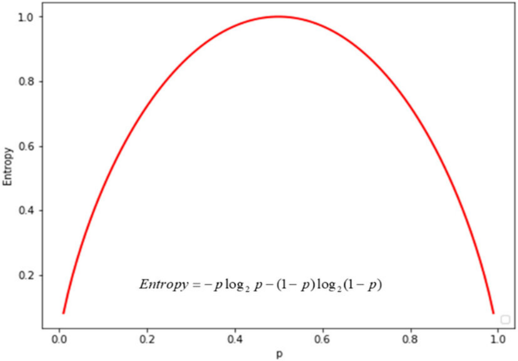

- $\sum_{v \in V(A)} \frac{|\mathcal{D}_v|}{|\mathcal{D}|} Entropy(\mathcal{D}_v)$ is weighted uncertainty of classes in each $\mathcal{D}_v$ (weighted by the relative size of $\mathcal{D}_v$).
- $Gain(\mathcal{D}, A)$ measures reduction in uncertainty of classes by splitting $\mathcal{D}$ according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

Gini Impurity

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

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

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

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

Gini Impurity

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

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

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

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

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

Example

Consider our tennis example (see the table).

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

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  - $Gini(\mathcal{D}) = 1 - (9/14)^2 - (5/14)^2 = 0.459$
- 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 $\mathcal{D} = \mathcal{D}_{Rain}$.

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

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

Attribute Importance Computation

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

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

There are several formulae for computing the importance.

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

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

Continuous-Valued Attributes

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

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

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

- τ is assigned a threshold value called a *cut point* $H \in \mathbb{R}$,
- there are two edges $e_{\text{true}}, e_{\text{false}}$ from τ,
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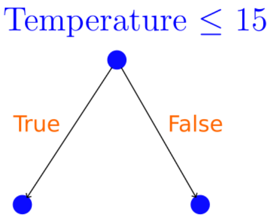
- there are two edges $e_{\text{true}}, e_{\text{false}}$ from τ,
- e_{true} labeled with True and e_{false} labeled with False.

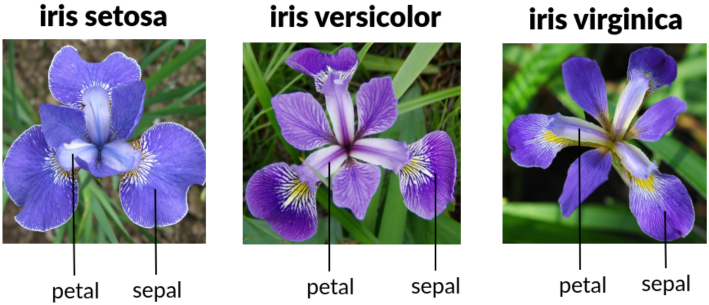
During inference, when considering an example $\vec{x}$ in the node τ,

- evaluate $A(\vec{x}) \leq H$,
- if $A(\vec{x}) \leq H$, then follow e_{true},
- else follow e_{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
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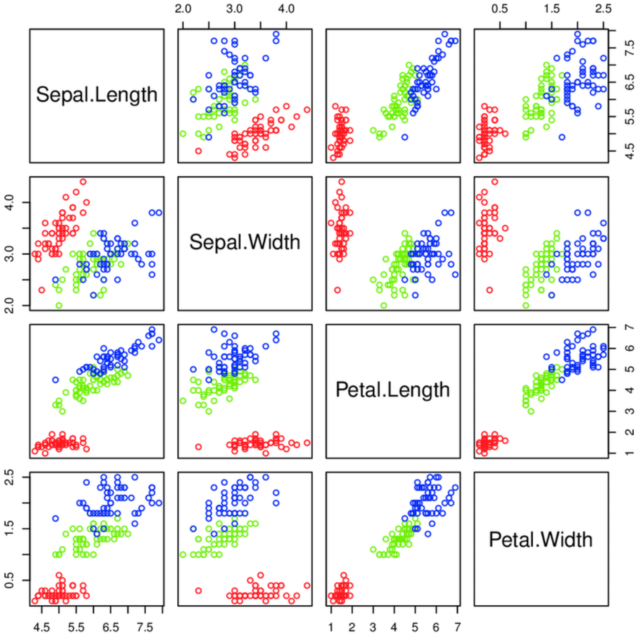
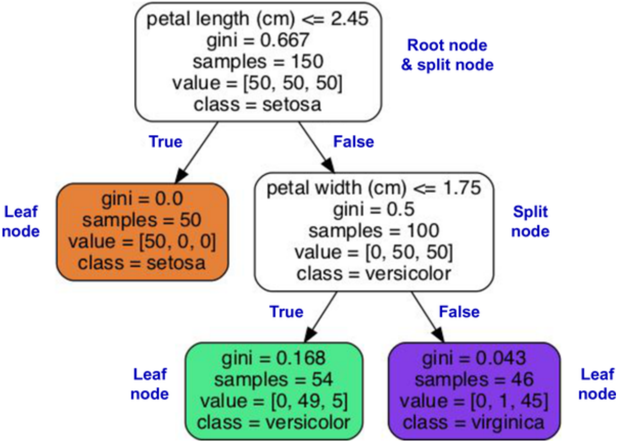
6.0	3.4	4.5	1.6	Versicolor
5.1	3.5	1.4	0.2	Setosa
6.6	3.0	4.4	1.4	Versicolor
5.9	3.2	4.8	1.8	Versicolor
5.6	2.8	4.9	2.0	Virginica
...				

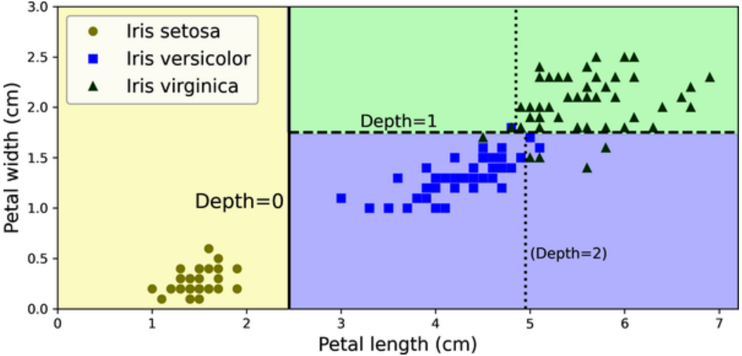
Iris Example



Iris Example - Decision Tree

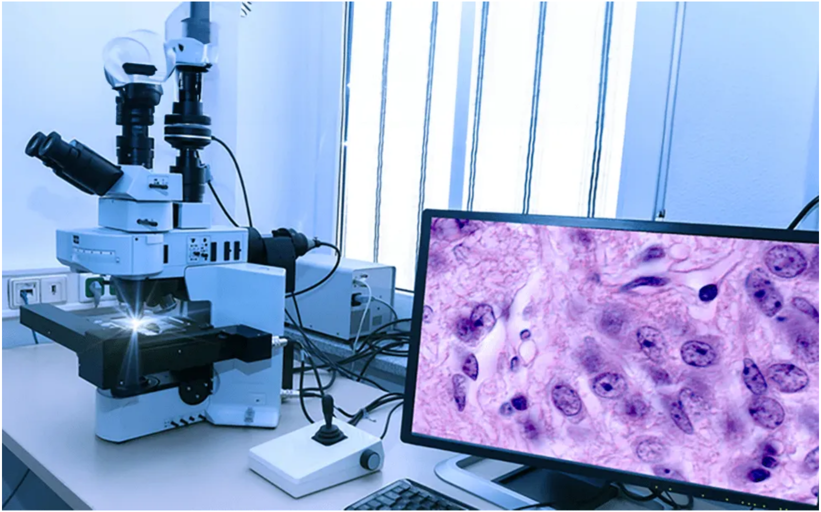


Iris Example - Decision Tree Boudaries



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

Example: Wisconsin Breast Cancer Dataset



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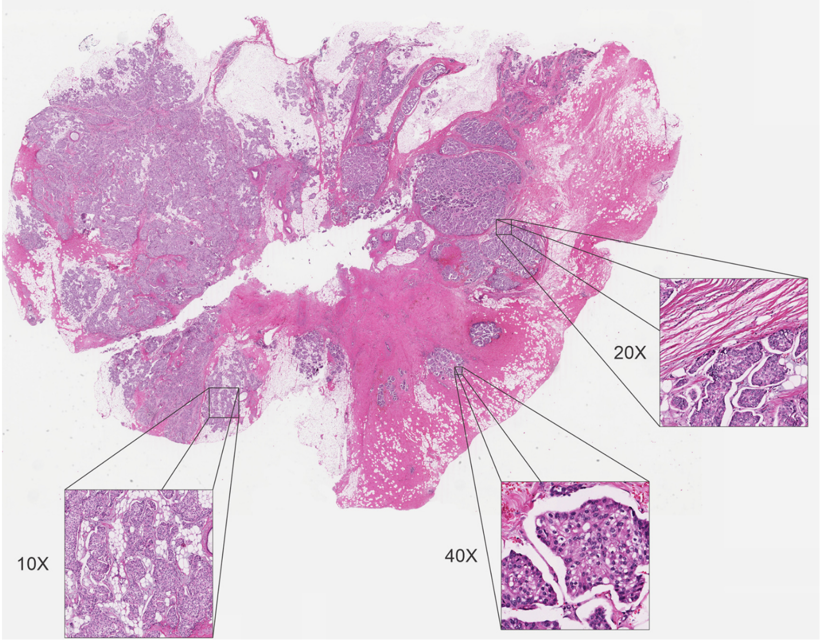

Example: Wisconsin Breast Cancer Dataset

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

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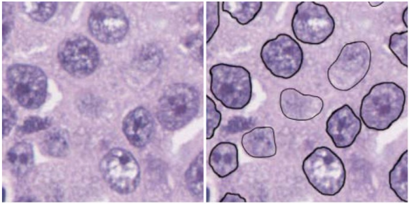

- Each sample is characterized by 10 different measurements:
  - Radius, Texture, Perimeter, Area
  - Smoothness, Compactness, Concavity
  - Concave Points, Symmetry, Fractal Dimension
- Each feature has three statistical measures:
  - Mean (Average over cells in the sample)
  - Standard Error (SE) (Variation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

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

Example: Wisconsin Breast Cancer Dataset

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

Example: Wisconsin Breast Cancer Dataset

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

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

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

I will:

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

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

Training Accuracy: 0.9956
Test Accuracy: 0.9474

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

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

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

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

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

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

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

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

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

Decision Trees

Practical Issues

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

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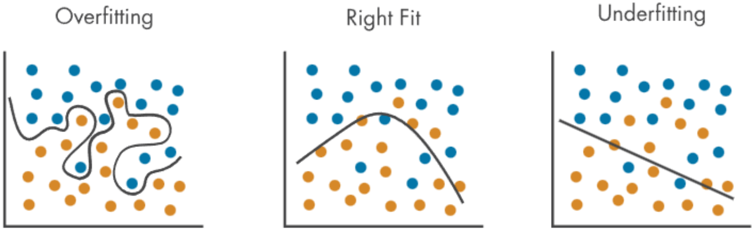
Imbalanced classes might cause problems because of small information gain/impurity decrease in splitting.

Model Tuning - Over/Under Fitting

The behavior of the model on the training set:



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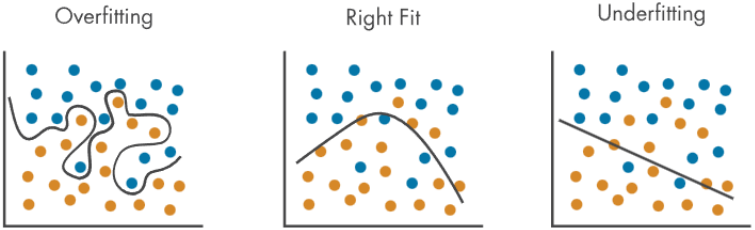

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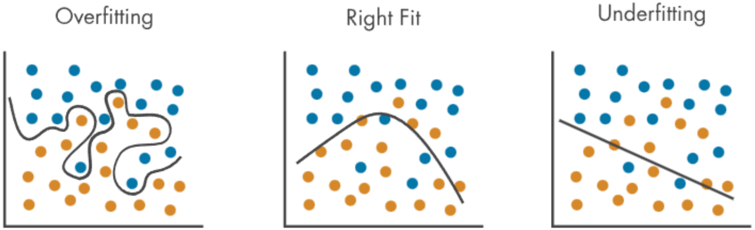

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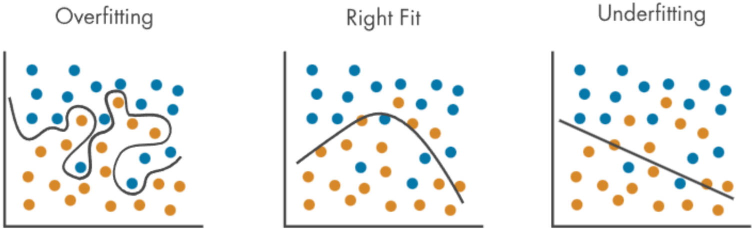

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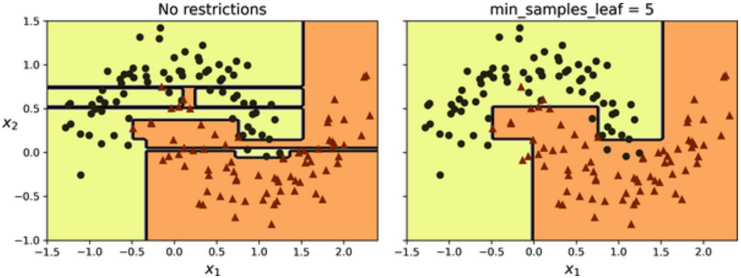
- The right one is strongly underfitting. It would probably give poor classification results.
- The middle one seems good (but still needs to be tested on fresh data).

Model Tuning - Overfitting in Decision Trees

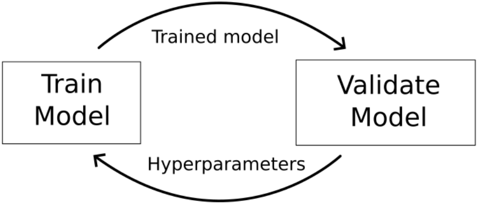


See the overfitting on the left and the "nice" model on the right.

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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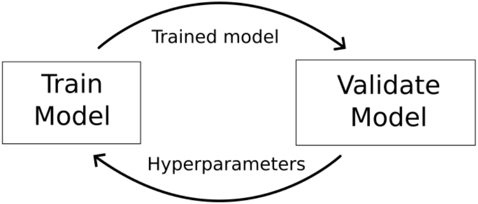

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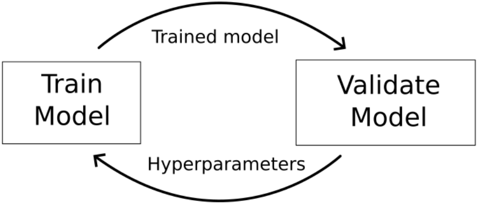

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What to observe? In the case of decision trees, one should observe the difference between performance measures (e.g., classification accuracy) on the training and validation sets.

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:

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

Post-Pruning - Reduced Error Pruning

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

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

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Train $\mathcal{T}$ to maximum fit on the *training dataset.*
while true **do**
  $Err[\mathcal{T}] \leftarrow$ the error of $\mathcal{T}$ on the validation set.
  for $\tau \in T_{int}$ **do**
    $Err[\mathcal{T}_{-\tau}] \leftarrow$ the error of $\mathcal{T}_{-\tau}$ on the validation set.
  end for
  if $Err[\mathcal{T}] \leq \min\{Err[\mathcal{T}_{-\tau}] \mid \tau \in T_{int}\}$] **then return** $\mathcal{T}$
  else
    $\mathcal{T} \leftarrow argmin\{Err[\mathcal{T}_{-\tau}] \mid \tau \in T_{int}\}$
  end if
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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  Typically introduce regularization into the error functions: Given a decision tree $\mathcal{T}$

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

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

Sensitivity to Small Changes and Randomness

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

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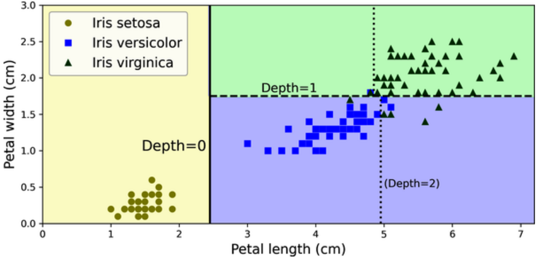
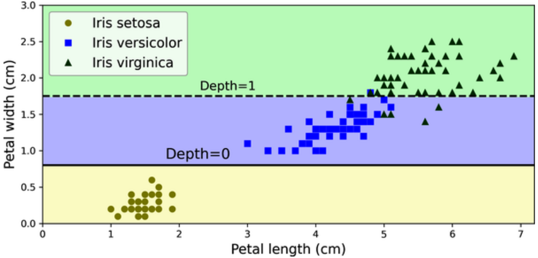
A solution is to train an ensemble of many decision trees and then use majority voting for classification.

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

Iris - Illustration



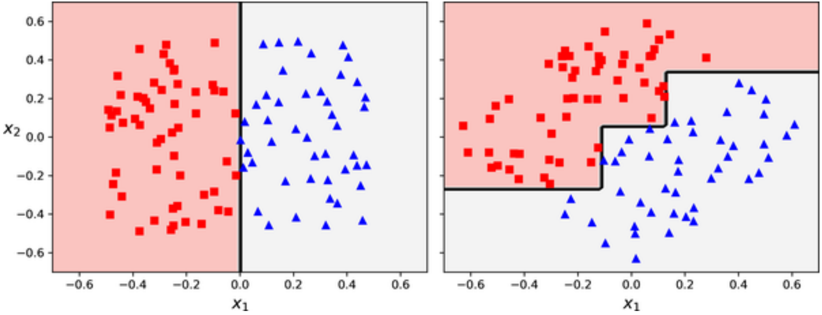


Decision trees trained on the Iris dataset.

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

Axis Sensitivity

The decision makes divisions along particular axes:

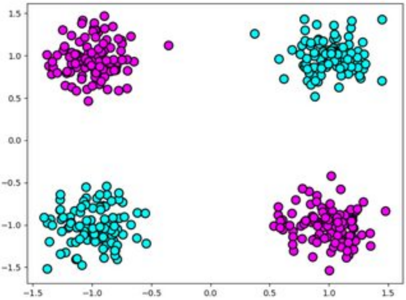


That is, rotated data may result in a completely different model.

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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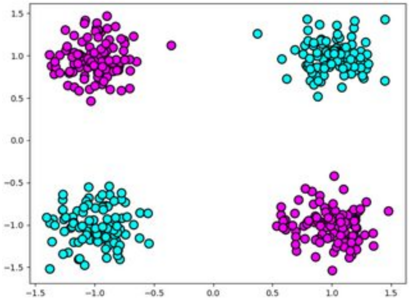
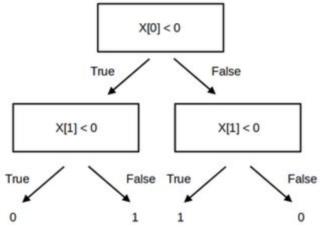
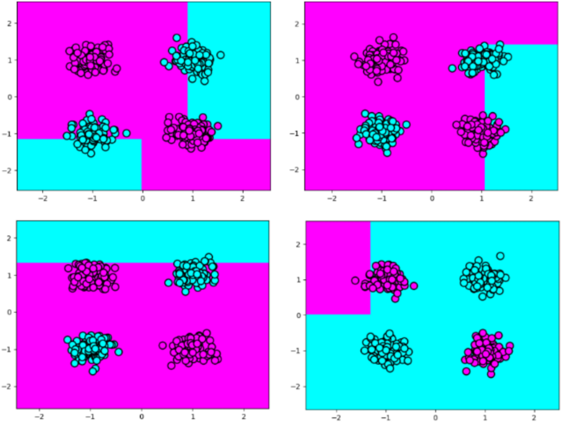


An ideal decision tree would look like this:



Attempts at Training on XOR

Max depth = 2:



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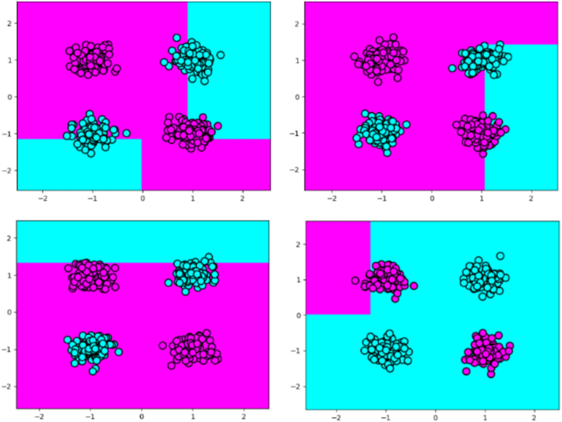
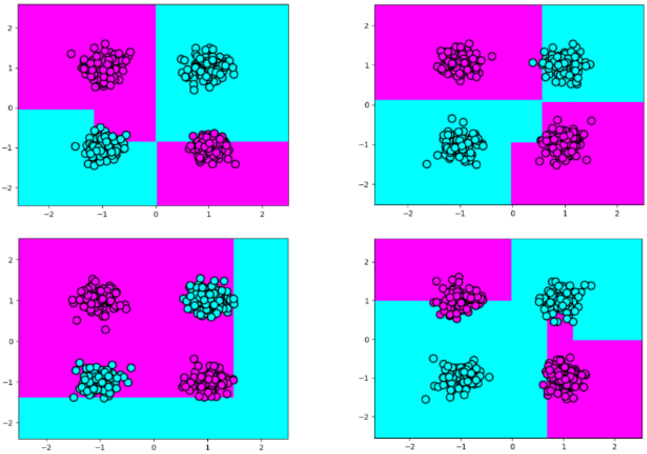


The problem: Both information gain and decrease in impurity consider only the relationship of a *single* attribute and the class.

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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- Not sensitive to outliers since the splitting is based on the proportion of examples within the split ranges and not on absolute values.
- 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.
- Non-smooth predictions: Decision trees make piecewise constant approximations, which are not suitable for extrapolation.

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- Difficulty learning certain concepts, such as XOR.
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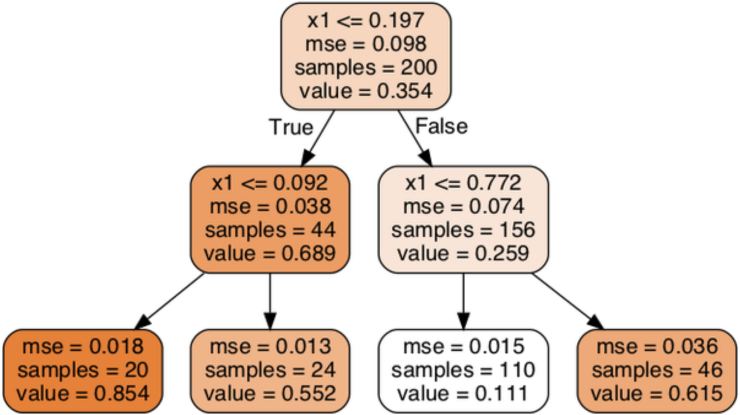
- Learning optimal trees is NP-complete: Heuristic algorithms like greedy algorithms are used, which do not guarantee globally optimal trees. Ensemble methods can help.

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.

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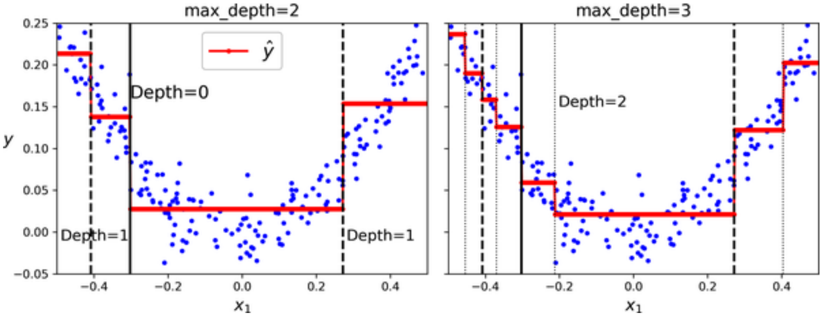

Intuitively, for every subinterval of x_1, the value (the red line) is at the average y over the subinterval.

How are the subintervals being set?

Regression Trees

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

We follow the same procedure as in decision trees during inference on an input $\vec{x}$.

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How exactly are such trees trained?

We aim to minimize the mean squared error.

Regression Trees

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

We follow the same procedure as in decision trees during inference on an input $\vec{x}$.

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

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

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

Minimizes the following *split error*:

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

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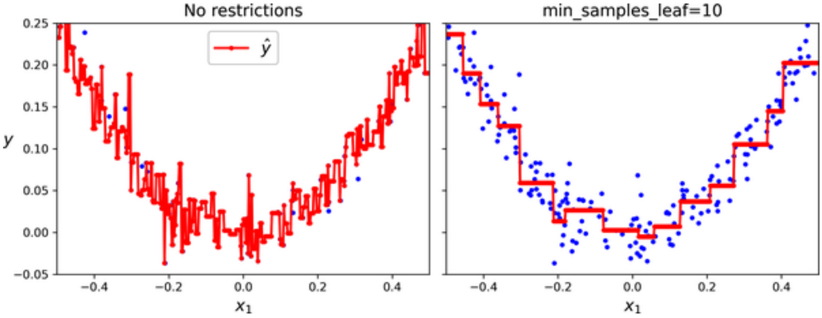
If Δ is large enough, split on A and H that minimize the split error. Otherwise, stop splitting and label the leaf with $\bar{\mathcal{D}}$.

Regression Tress

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



Probabilistic Classification

Probabilistic Classification – Idea

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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 Ω of *possible outcomes*, Ω is called *sample space*.

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

$$P(E) = \sum_{\omega \in E} f(\omega)$$

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

Conditional Probability and Independence

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

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

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

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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: $X : \{1, \ldots, 6\} \to \{0, 1\}$ 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 Ω 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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"Summing over" all possible values of some variable(s) gives the distribution of the rest:

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

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

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

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

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

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

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

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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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...			

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

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

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

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Proof.

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

□

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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

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

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

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

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

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We introduce *independence assumptions* about the features!

Naive Bayes

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

$$
\begin{aligned}
P(X = x \mid Y = y) &= P(X_1 = x_1, \cdots, X_n = x_n \mid Y) \\
&= \prod_{i=1}^{n} P(X_i = x_i \mid Y = y)
\end{aligned}
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- Therefore, we only need to specify $P(X_i = x_i \mid Y = y)$ for each possible pair of a feature-value x_i and $y \in \{\mathbf{0}, \mathbf{1}\}$.

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

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

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

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

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

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

Y	X_1	X_2	X_3
1	1	0	1
1	0	1	1
0	1	0	1
0	0	0	1
1	0	0	0
0	1	1	1

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

Naive Bayes – Example

Consider classification of geometric shapes:

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

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

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

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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
$\bar{P}(red \mid Y)$	0.9	0.3
$\bar{P}(circle \mid Y)$	0.9	0.3

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

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

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

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$$\doteq 0.5 \cdot 0.2 \cdot 0.3 \cdot 0.3 \,/\, P(X=\vec{x}) = 0.009/P(X=\vec{x})$$

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

	$Y = \mathbf{1}$	$Y = \mathbf{0}$
$\bar{P}(Y)$	0.5	0.5
$\bar{P}(medium \mid Y)$	0.1	0.2
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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.)
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

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

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

But then $\bar{P}(X = x) = 0$ for x containing the value x_i for X_i, and thus $\bar{P}(Y = y \mid X = x)$ is not well defined.
Moreover, $\bar{P}(Y = y) \cdot \bar{P}(X = x \mid Y = y) = 0$ (for $y \in \{\mathbf{0}, \mathbf{1}\}$) so even this cannot be used for classification.

Probability Estimation Example

Training data:

Size	Color	Shape	Class
small	red	circle	**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*.

Smoothing

- 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

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

To understand note that

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

and thus

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

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

Laplace Smoothing Example

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

Continuous Features

Ω 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

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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 μ_{iy} and the standard deviation σ_{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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- Directly constructs a model from parameter estimates that are calculated from the training data.
- Typically handles outliers and noise well in the discrete version. In the continuous case depends on the way the parameters are estimated (e.g., the mean is very sensitive to outliers).
- Missing values are easy to deal with; use only non-missing values in the computation of $\bar{P}(X_i = x_i \mid Y = y)$.

Bayesian Networks (Basic Information)

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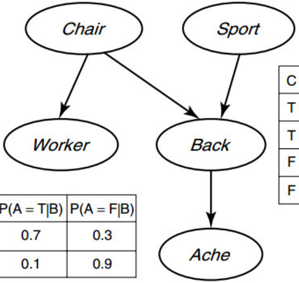
Bayesian networks are a graphical model that uses a directed acyclic graph to specify dependencies among variables.

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)
T	0.9	0.1
F	0.01	0.99

C	S	P(B = T|C,S)	P(B = F|C,S)
T	T	0.9	0.1
T	F	0.2	0.8
F	T	0.9	0.1
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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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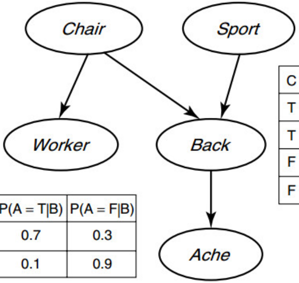

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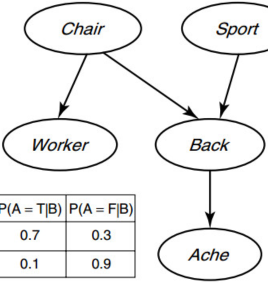

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Now, we may, e.g., infer the probability $P(C = T \mid A = T)$ that we sit in the wrong chair, assuming that our back aches.
We have to store only 10 numbers as opposed to $2^5 - 1$ possible probabilities for all vectors of values of C, S, W, B, A.

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

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

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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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Confusion Matrix for Binary Classifier

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Example

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:

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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
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Result	FN	FN	TP	TP	TP	TP	TP	TP	FP	TN	TN	TN

Actual condition	**Predicted condition**	
	Cancer	**Non-cancer**
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Terminology

- TP aka hit
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In what follows, we also use

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Note that $\mathrm{P} + \mathrm{N} = \mathrm{PP} + \mathrm{PN}$ is the number of all cases.

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

Accuracy

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

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$$\text{Precision} = 1$$

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

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

Precision & Recall - Relative Importance

Let us get back to our cancer example:

Actual condition	**Predicted condition**	
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Consider *Precision* and *Recall*.

By now, you should remember what they measure.

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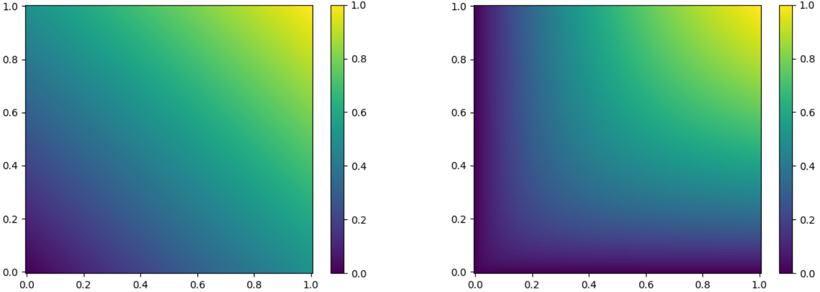
Compare the arithmetic (left) and harmonic (right) mean:



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

Consider the cancer example:

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

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Our imbalanced example:

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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.

Imbalanced Classes Once More

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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.

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

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 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
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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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For a given class $i \in C$:

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

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

Example

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

Compute the metrics.

Example

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

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

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

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

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

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

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

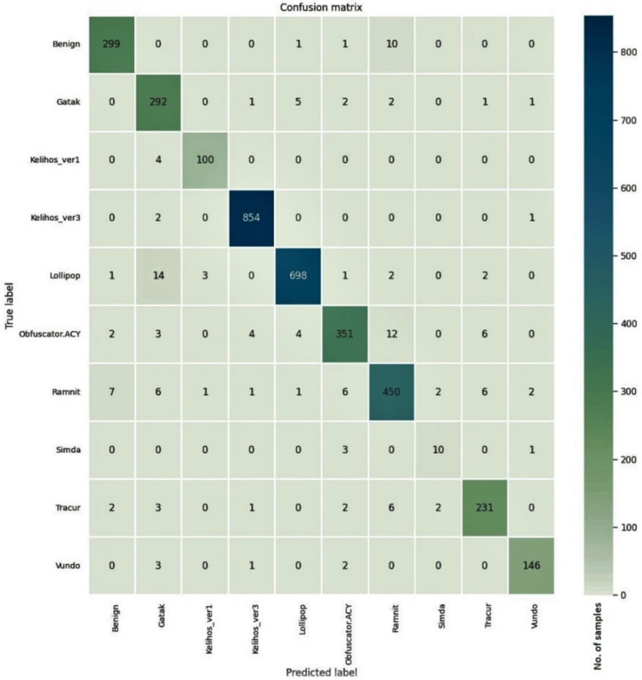
Actual	**Predicted**		
	big	**medium**	**small**
big	5	0	1
medium	0	2	2
small	1	1	3

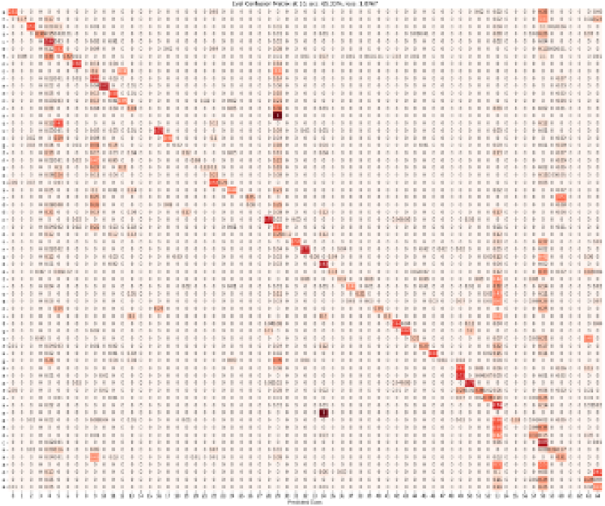
$$F_1[\text{big}] = \frac{2 * (5/6) * (5/6)}{(5/6) + (5/6)} = 5/6 = 0.83$$

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

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

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
299 0 0 0 1 1 10 0 0 0
0 292 0 1 5 2 2 0 1 1
0 4 100 0 0 0 0 0 0 0
0 2 0 854 0 0 0 0 0 1
1 14 3 0 698 1 2 0 2 0
2 3 0 4 4 351 12 0 6 0
7 6 1 1 1 6 450 2 6 2
0 0 0 0 0 3 0 10 0 1
2 3 0 1 0 2 6 2 231 0
0 3 0 1 0 2 0 0 0 146
800
700
600
500
400
300
200
100
0



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 sequence of predictions generated by a classifier.
Now the classifier returns *probability of class* 1 for a given input:

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

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 $h_1, \dots, h_p$?

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

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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We obtain

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

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and

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and

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

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

Thresholded Classifier Metrics

Index	1	2	3	4	5	6	7	8	9	10	11	12
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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

Thresholded Classifier Metrics

Index	1	2	3	4	5	6	7	8	9	10	11	12
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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

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

Thresholded Classifier Metrics

Index	1	2	3	4	5	6	7	8	9	10	11	12
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$$\text{TP}[T] = 6 \quad \text{FP}[T] = 2 \quad \text{FN}[T] = 1 \quad \text{TN}[T] = 3$$

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

Thresholded Classifier Metrics

Index	1	2	3	4	5	6	7	8	9	10	11	12
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$$\text{Accuracy}[T] = \frac{3+6}{12} \quad \text{Precision}[T] = \frac{6}{6+2} \quad \text{Recall}[T] = \frac{6}{6+1}$$

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

Receiver Operating Characteristic (ROC)

Consider two metrics for a given T:

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

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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.

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

Index	1	2	3	4	5	6	7	8	9	10	11	12
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- $0.00 \leq T \leq 0.05$: TPR $= 1$ and FPR $= 1$
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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
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Index	1	2	3	4	5	6	7	8	9	10	11	12
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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
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- $0.42 < T \leq 0.43$: TPR $= 5/7$ and FPR $= 2/5$
- $0.43 < T \leq 0.48$: TPR $= 5/7$ and FPR $= 1/5$

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

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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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- $0.90 < T \leq 0.95$: TPR $= 2/7$ and FPR $= 0$
- $0.95 < T \leq 0.98$: TPR $= 1/7$ and FPR $= 0$

Index	1	2	3	4	5	6	7	8	9	10	11	12
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- $0.15 < T \leq 0.36$: TPR $= 1$ and FPR $= 2/5$
- $0.36 < T \leq 0.42$: TPR $= 6/7$ and FPR $= 2/5$
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- $0.43 < T \leq 0.48$: TPR $= 5/7$ and FPR $= 1/5$
- $0.48 < T \leq 0.66$: TPR $= 5/7$ and FPR $= 0$
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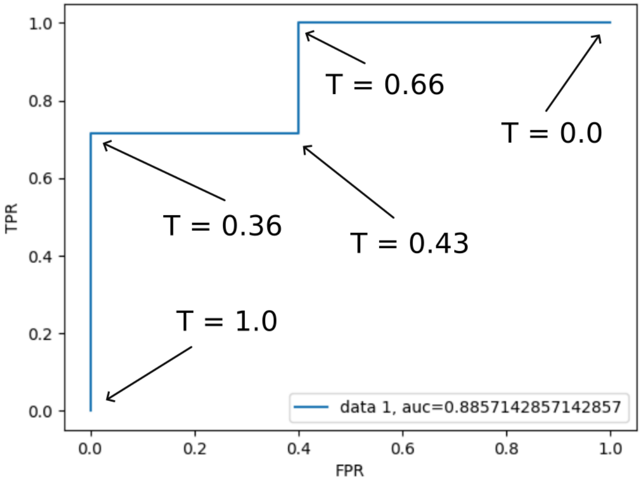
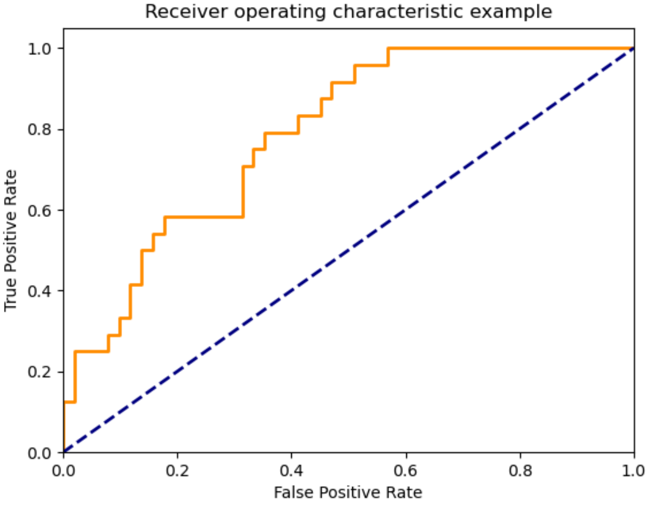
ROC

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

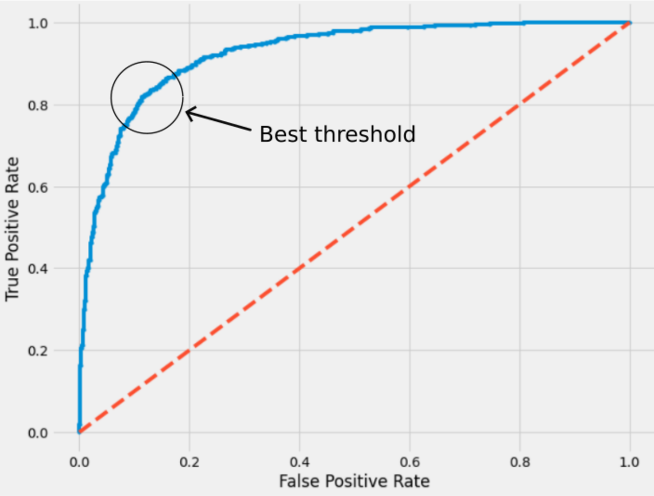


Iris Dataset - A Classifier



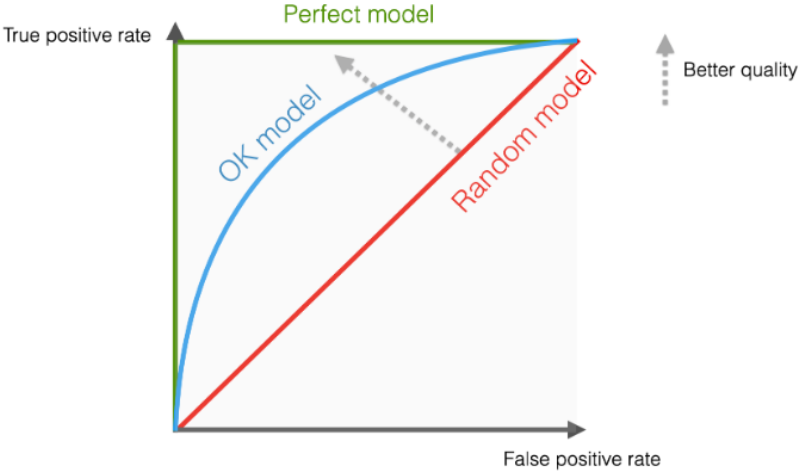
Example from the scikit-learn manual - SVM classifier trained in Iris

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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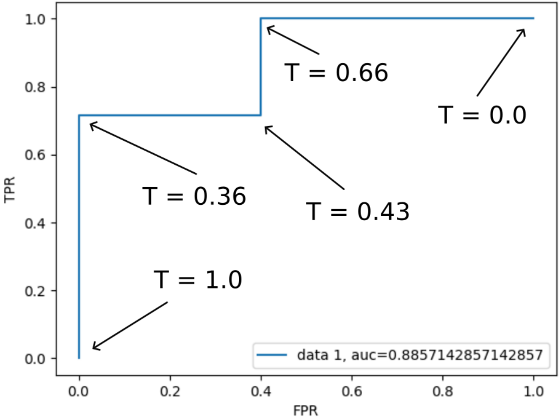
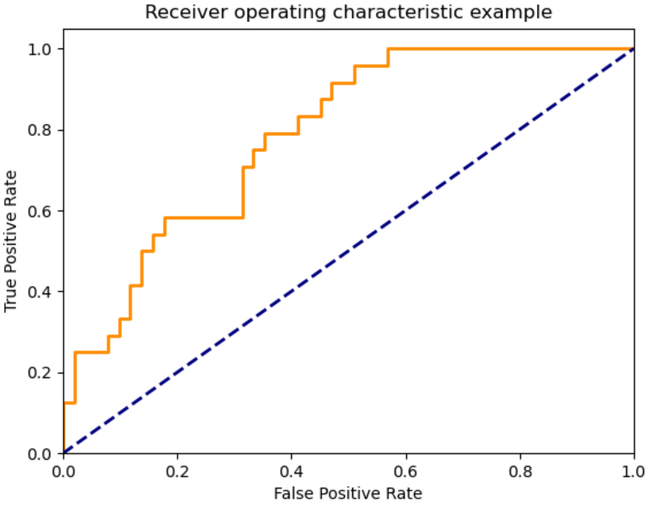


ROC-AUC $= 0.8857$

Iris - ROC-AUC



ROC-AUC = 0.79

ROC-AUC - Probabilistic Interpretation

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

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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:

- **Final test**: Evaluate the model on the test set (separated at the beginning of training) and then compute the metrics. May inform the user about the quality of the model.

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  There are (at least) two scenarios in which this happens:
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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.

How to Estimate Significance

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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.

How to Compare Classifiers

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Thresholding

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

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

- 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 $5/8$.

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

Linear Models

Numerical features

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

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- Most non-numerical features can be conveniently transformed to numerical ones.

  For example:
  - Colors $\{blue, red, yellow\}$ can be represented by

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

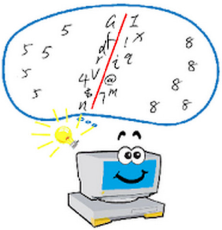
    (one-hot encoding)
  - Words can be embedded into vector spaces by various means (word2vec etc.)
  - A black-and-white picture of $x \times y$ pixels can be encoded as a vector of xy numbers that capture the shades of gray of the pixels.
    (Even though this is not the best way of representing images.)

Basic Problems

We consider two basic problems:

- (Binary) classification

  Our goal: Classify inputs into two categories.



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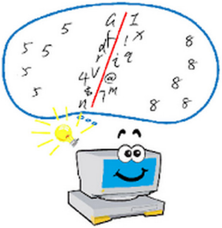
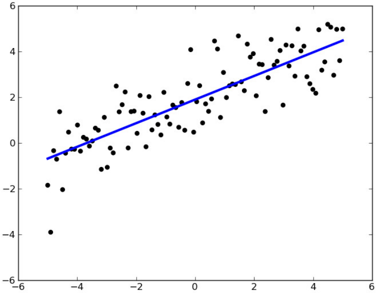


- Regression

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



Linear Models

Binary Classification

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

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Comments:

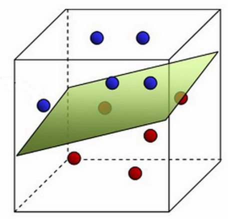
- In practice, we often do not strictly demand $h(\vec{x}) = c$ for all training examples $(\vec{x}, c) \in D$ (often it is impossible)
- We are more interested in good **generalization**, that is how well h classifies new instances that do not belong to D.

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

Models

We consider two kinds of models:

- Linear (affine) classifiers (this lecture)



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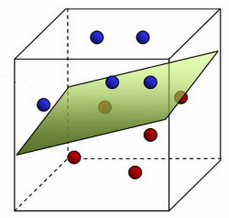
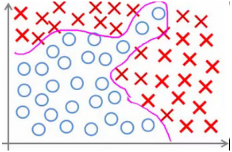
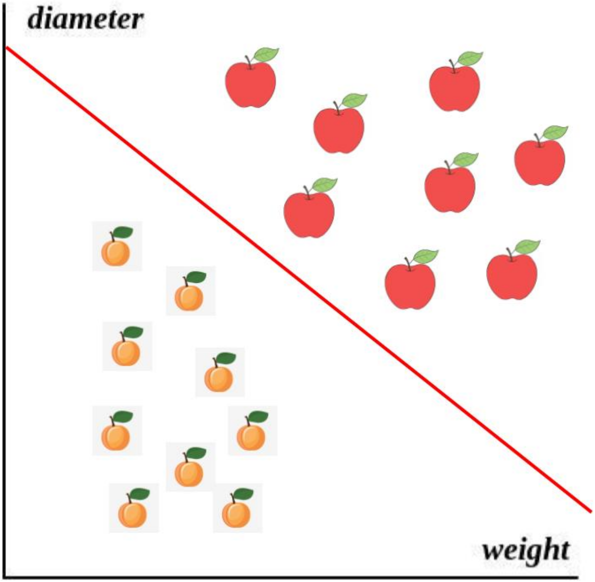


- Non-linear classifiers (kernel SVM, neural networks) (later lectures)



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

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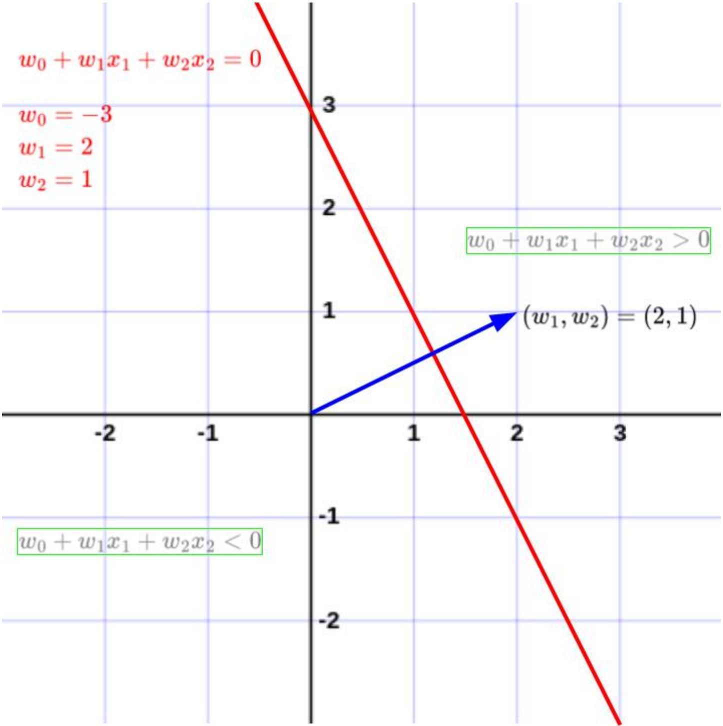
More succinctly:

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

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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3
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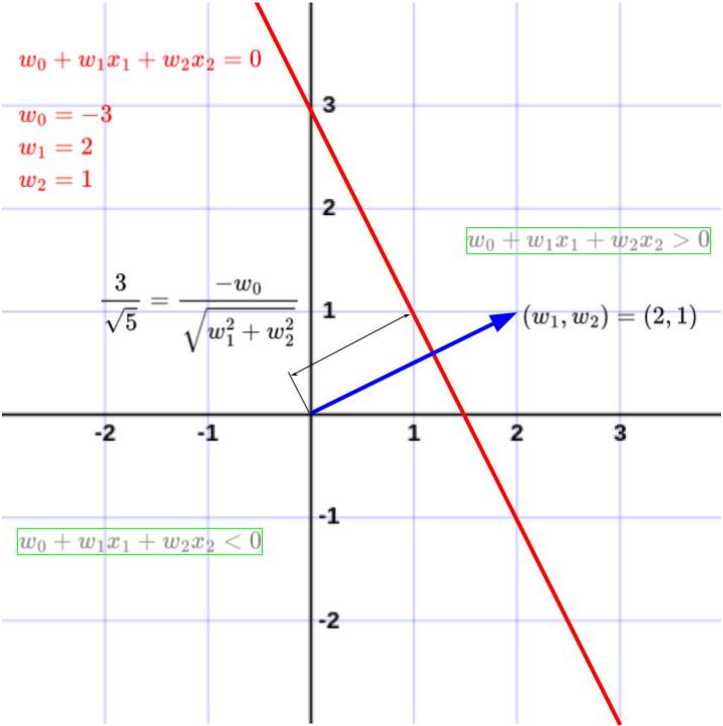

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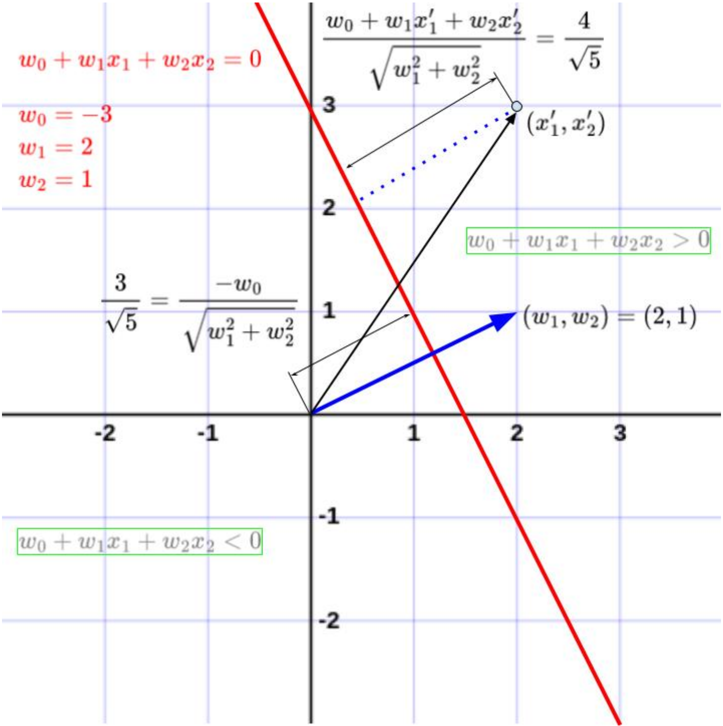

$\frac{w_0 + w_1 x'_1 + w_2 x'_2}{\sqrt{w_1^2 + w_2^2}} = \frac{4}{\sqrt{5}}$
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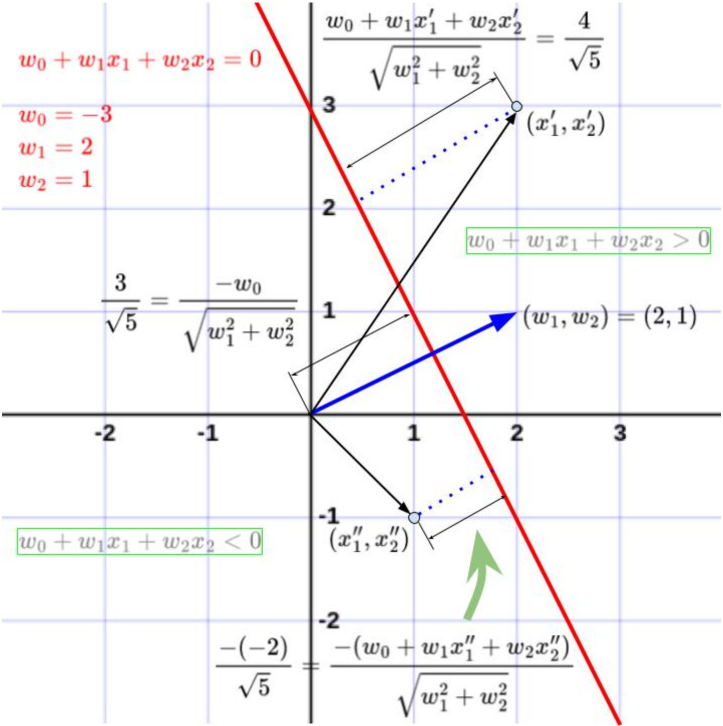

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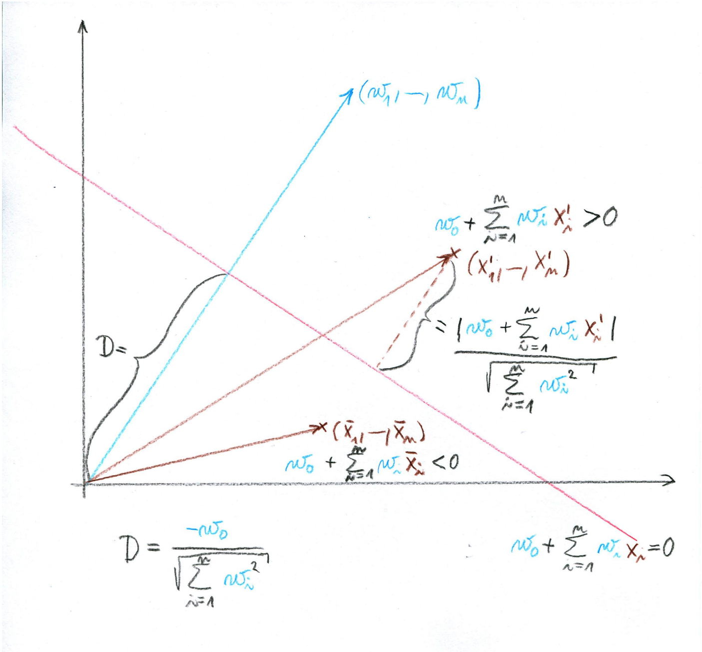
$w_0 + w_1 x_1 + w_2 x_2 < 0$
$\frac{-(-2)}{\sqrt{5}} = \frac{-(w_0 + w_1 x_1'' + w_2 x_2'')}{\sqrt{w_1^2 + w_2^2}}$

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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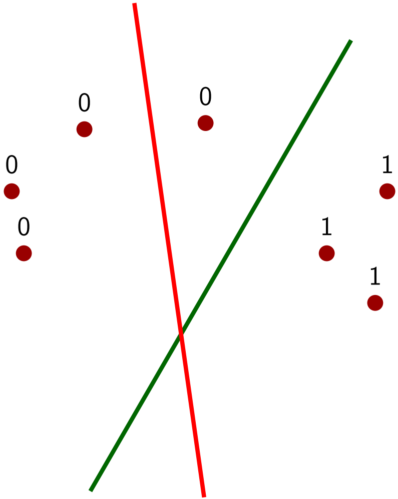
This makes the notation for the linear classifier more succinct:

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

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

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

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

Perceptron – Learning Algorithm

Online learning algorithm:

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

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

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

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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:

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

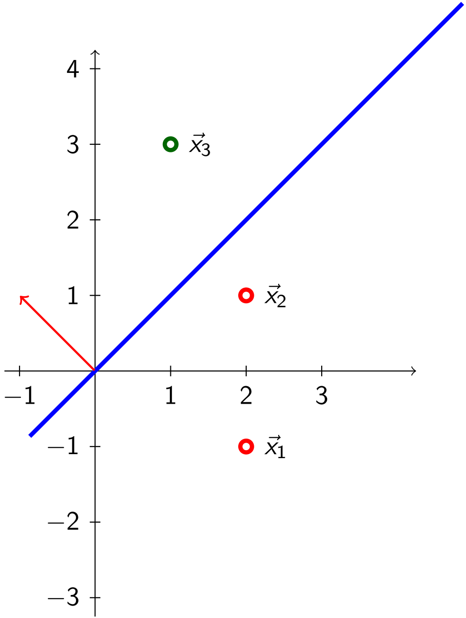
That is

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

$$c_1 = 1$$
$$c_2 = 1$$
$$c_3 = 0$$

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

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



Denoting $\vec{w}^{(0)} = (w_0, w_1, w_2) = (0, -1, 1)$ the blue separating line is given by $w_0 + w_1 x_1 + w_2 x_2 = 0$.

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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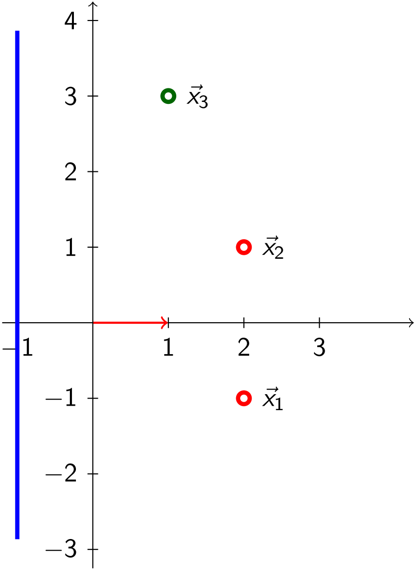


Example: Computing $\vec{w}^{(2)}$

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

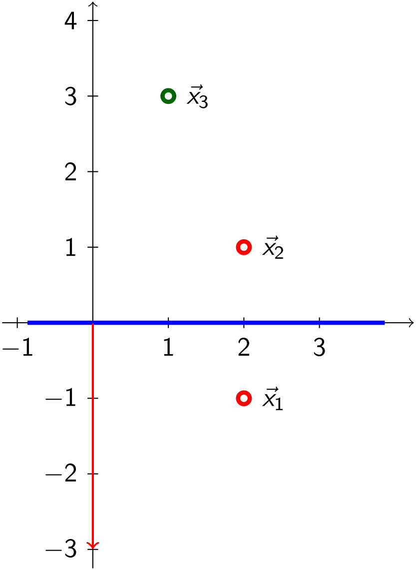
$$sgn\left(\vec{w}^{(2)} \cdot \tilde{\mathbf{x}}_3\right) - c_3 = 1 - 0 = 1$$

(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

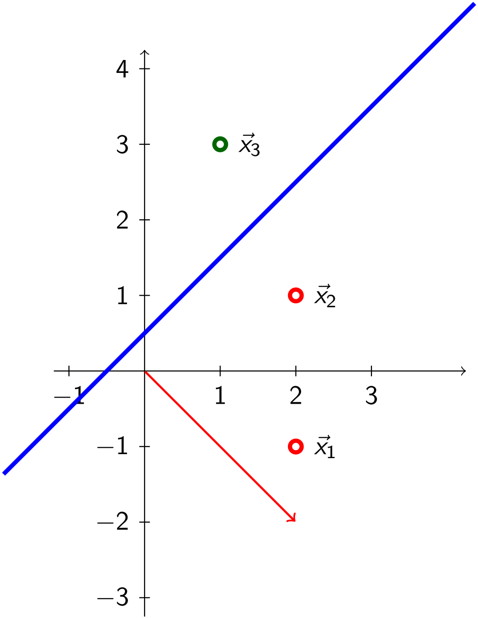
$$sgn\left(\vec{w}^{(4)} \cdot \tilde{\mathbf{x}}_2\right) - c_2 = 0 - 1 = -1$$

(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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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
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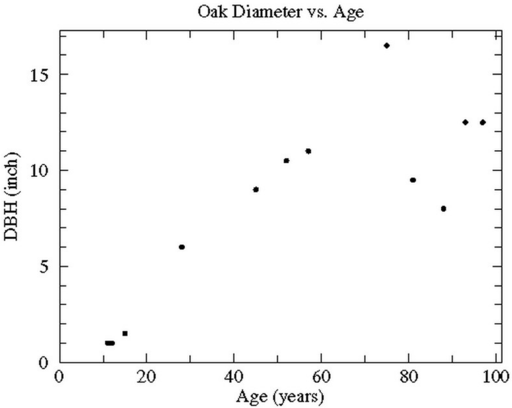

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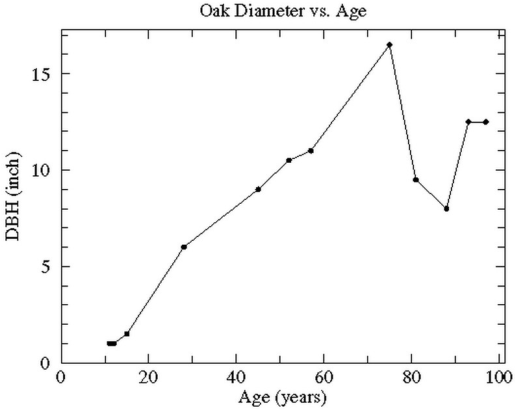

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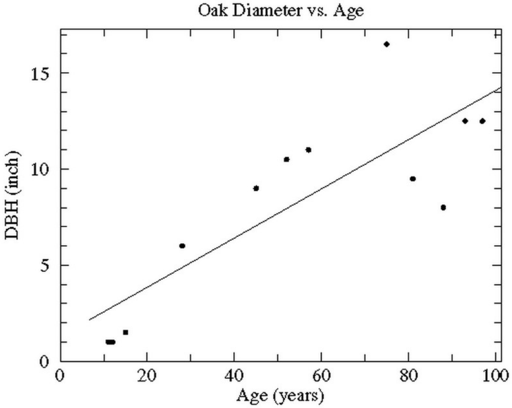

possibly YES!

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  Also called *loss function*.

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

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

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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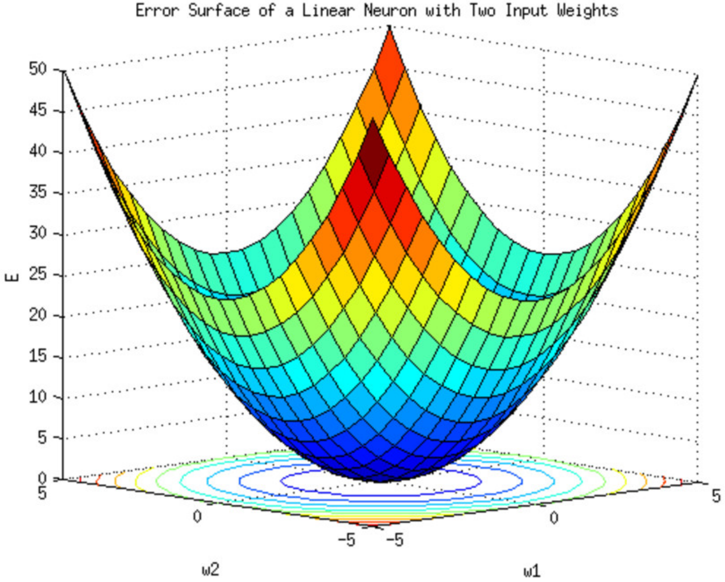
- **Squared Error Function:**

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

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!

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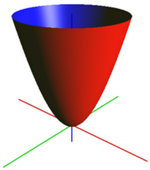
Fact:
If $\nabla E(\vec{w}) = \vec{0} = (0, \ldots, 0)$, then $\vec{w}$ is a global minimum of E.

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



Gradient of the error function

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

Then the model is $h[\vec{w}](x) = w_0 + w_1 \cdot x$.

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

Function Approximation – Learning

Gradient Descent:

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

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

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Proposition

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

Training set:

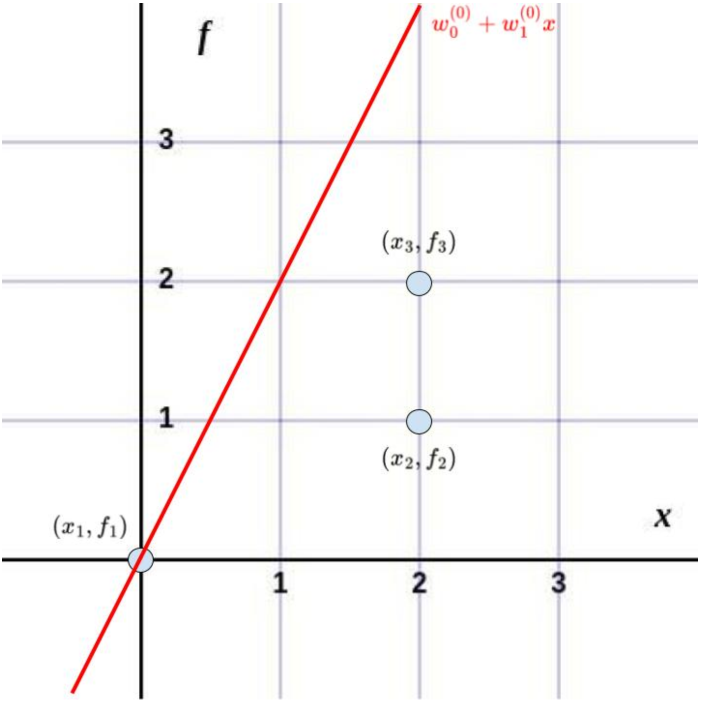
$$D = \{(x_1, f_1), (x_2, f_2), (x_3, f_3)\} = \{(0, 0), (2, 1), (2, 2)\}$$

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

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

$$f_1 = 0$$
$$f_2 = 1$$
$$f_3 = 2$$

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


$w_0^{(0)} + w_1^{(0)} x$
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: $\tilde{\mathbf{x}}_1 = (1,0)$, $\tilde{\mathbf{x}}_2 = (1,2)$, $\tilde{\mathbf{x}}_1 = (1,2)$

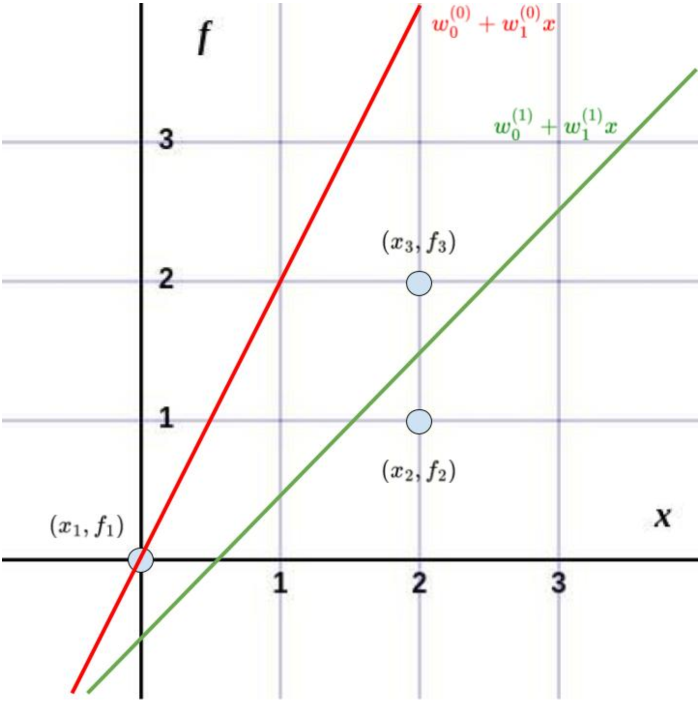
$$\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \frac{\partial E}{\partial w_1}(\vec{w})\right) = (w_0 + w_1 \cdot x_1 - f_1) \cdot \tilde{\mathbf{x}}_1$$
$$+ (w_0 + w_1 \cdot x_2 - f_2) \cdot \tilde{\mathbf{x}}_2$$
$$+ (w_0 + w_1 \cdot x_3 - f_3) \cdot \tilde{\mathbf{x}}_3$$

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

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



$w_0^{(0)} + w_1^{(0)} x$
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f
x
3
2
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(x_3, f_3)
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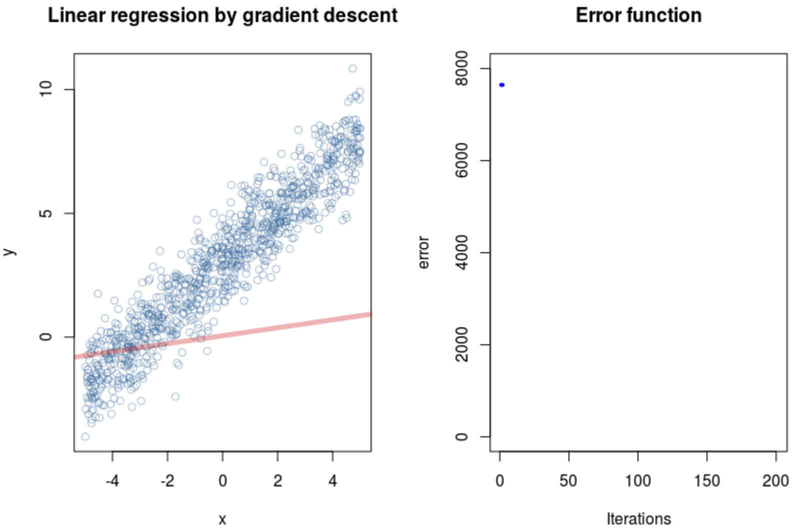
Linear Regression - Animation



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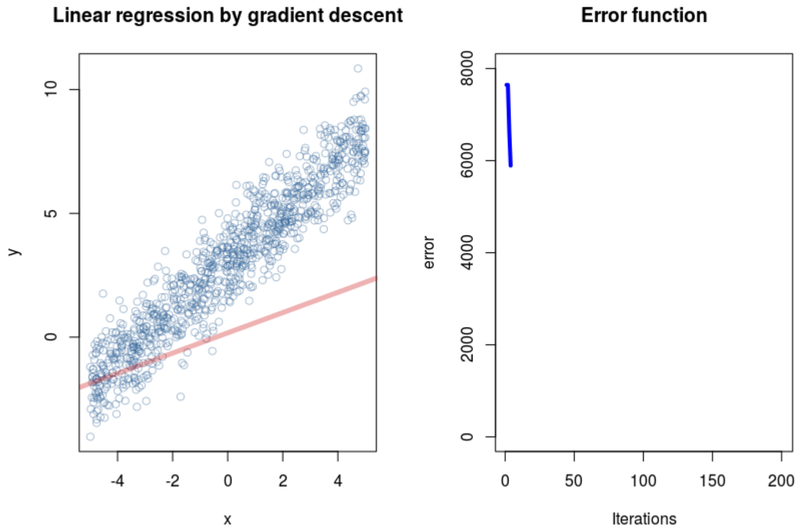

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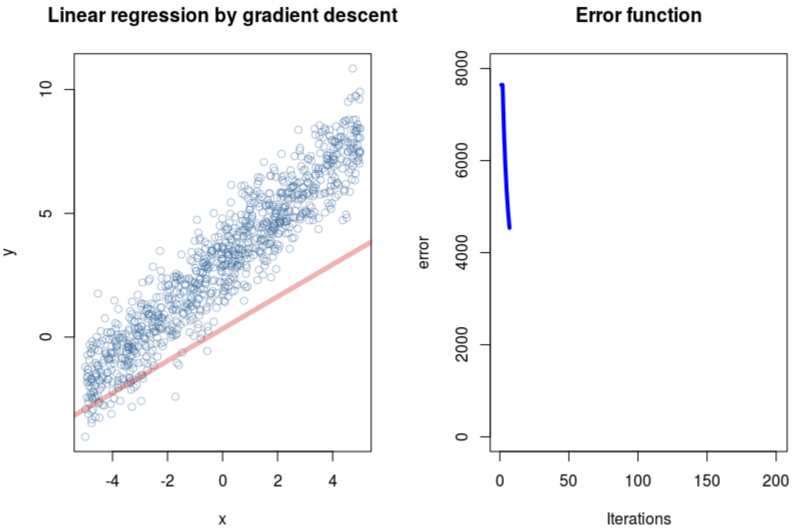

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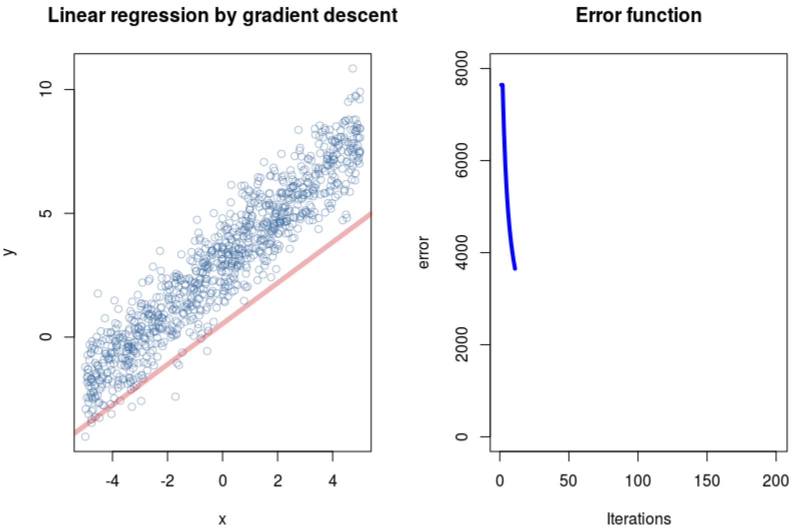

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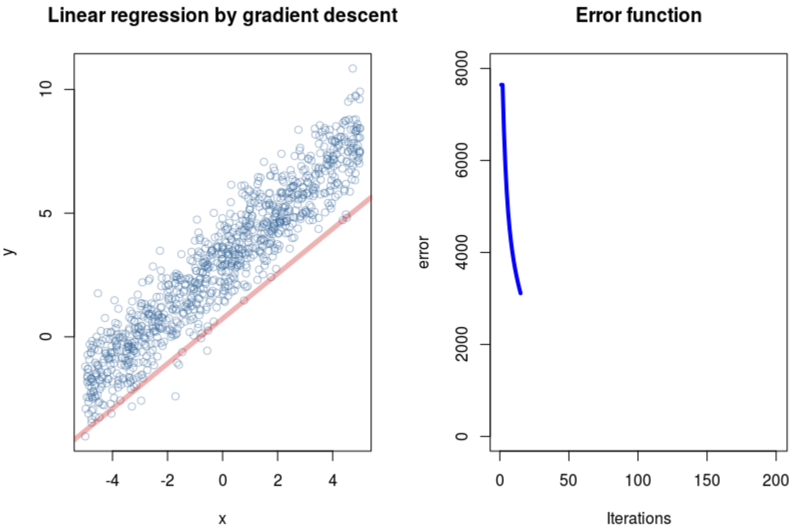

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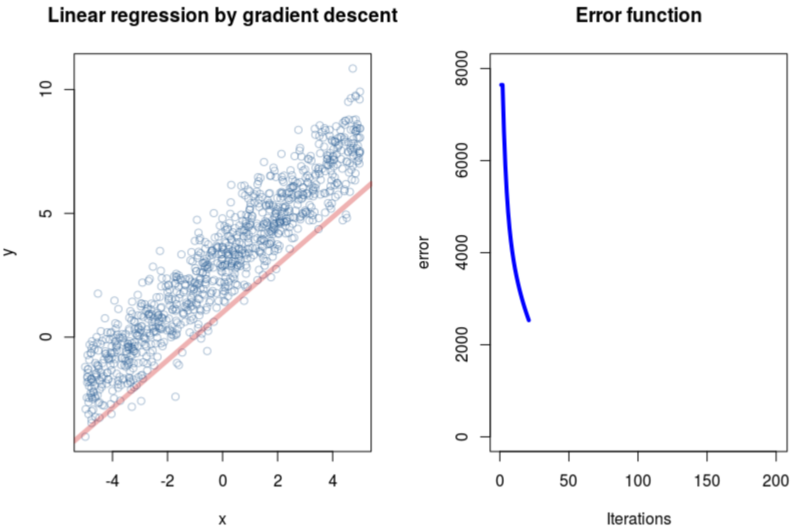

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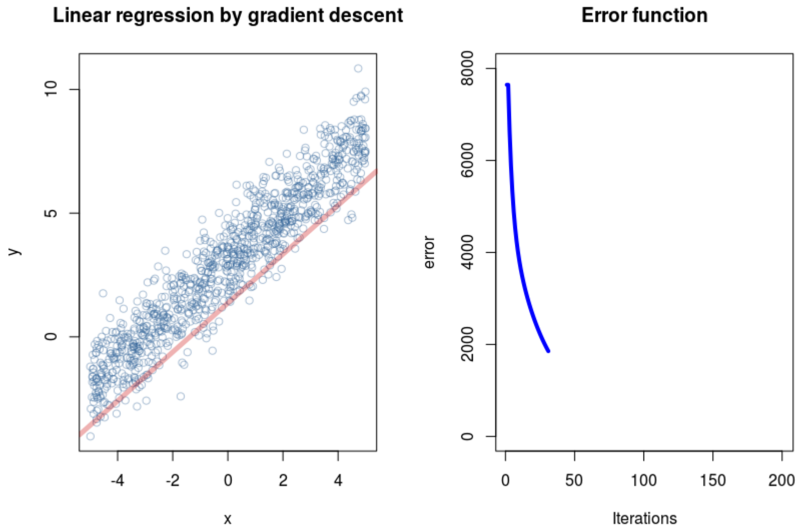

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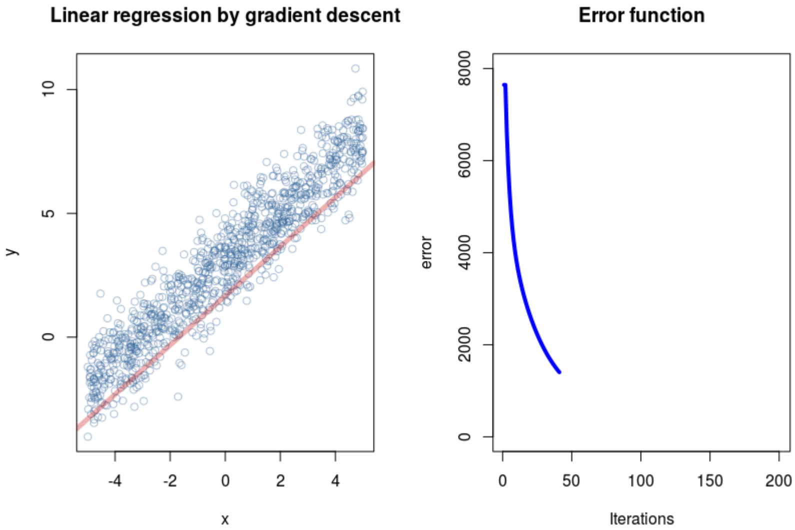

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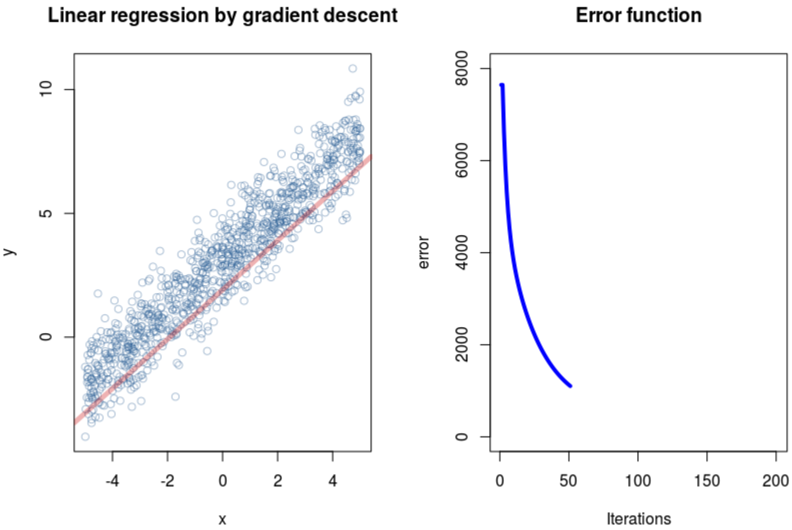

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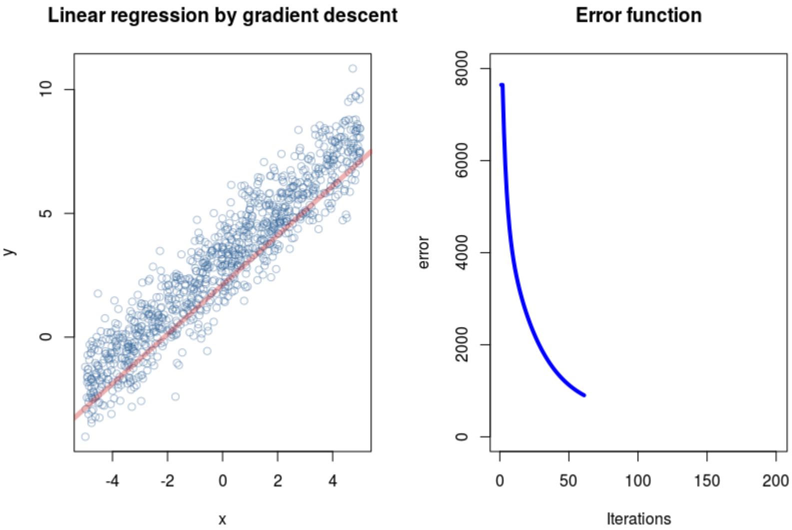

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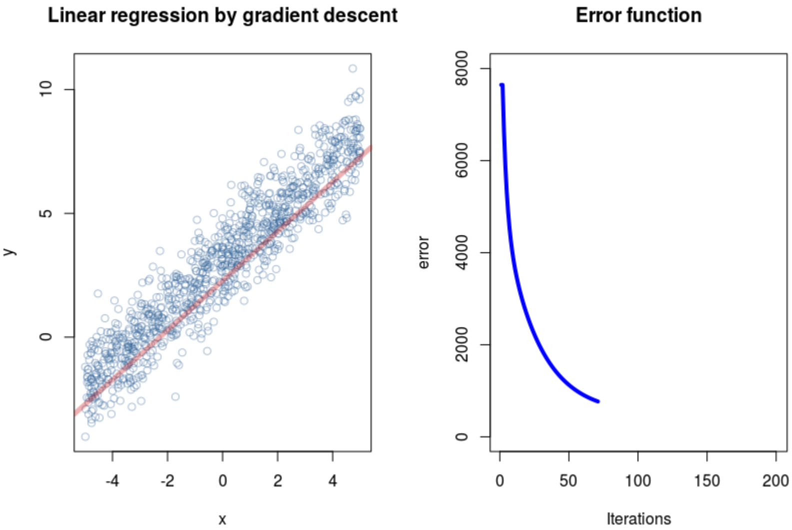
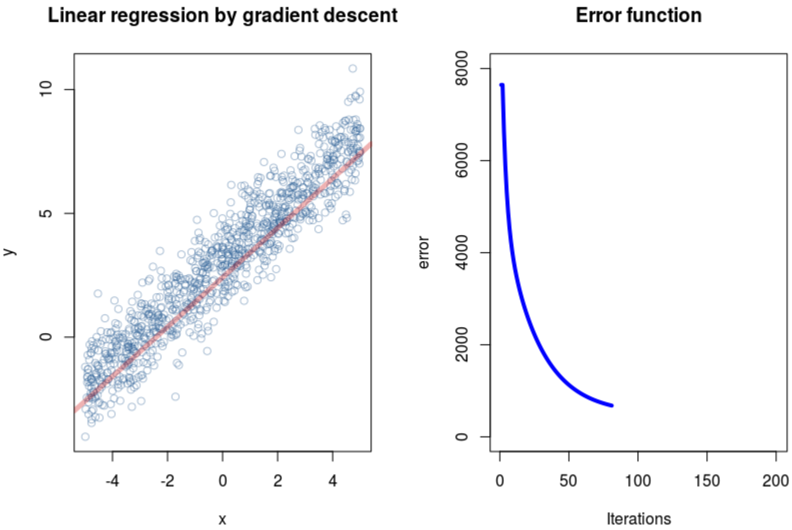
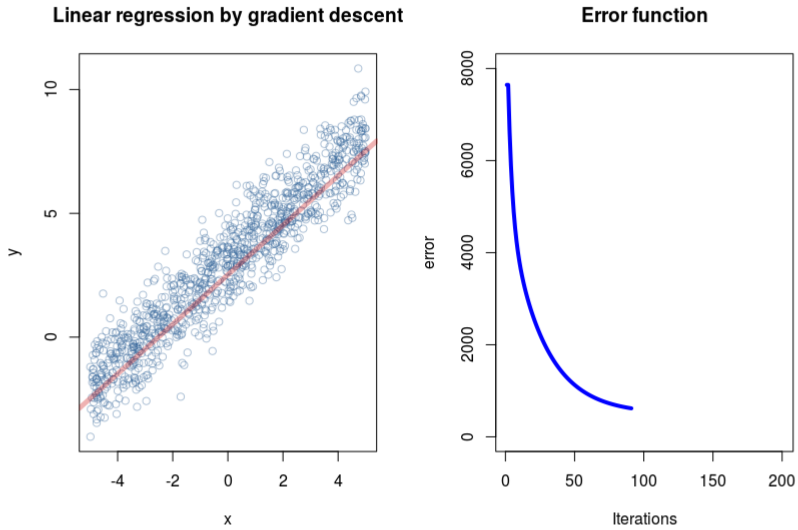


Linear Regression - Animation



Linear Regression - Animation



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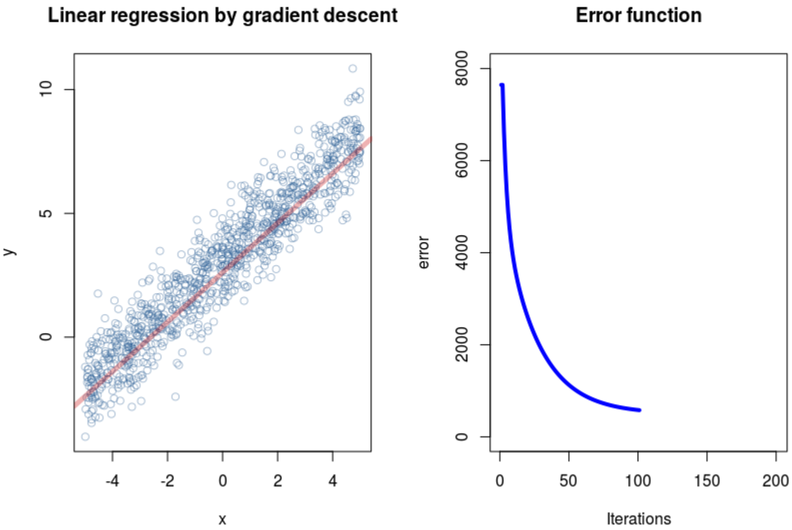

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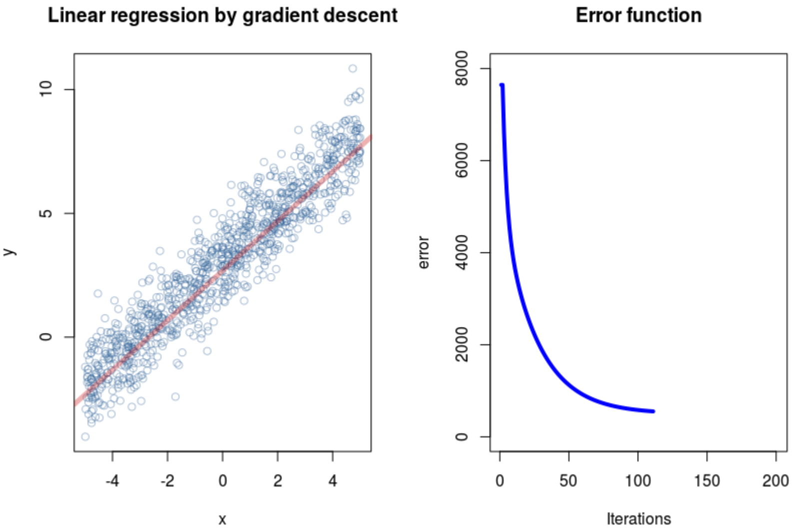

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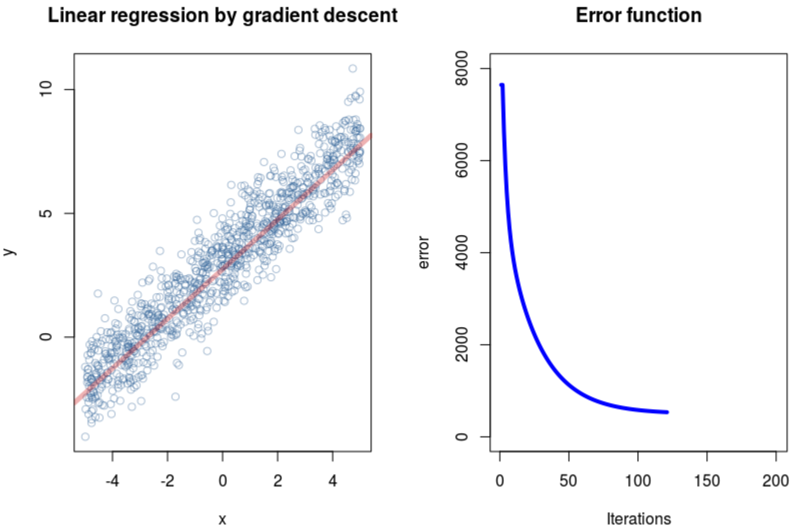

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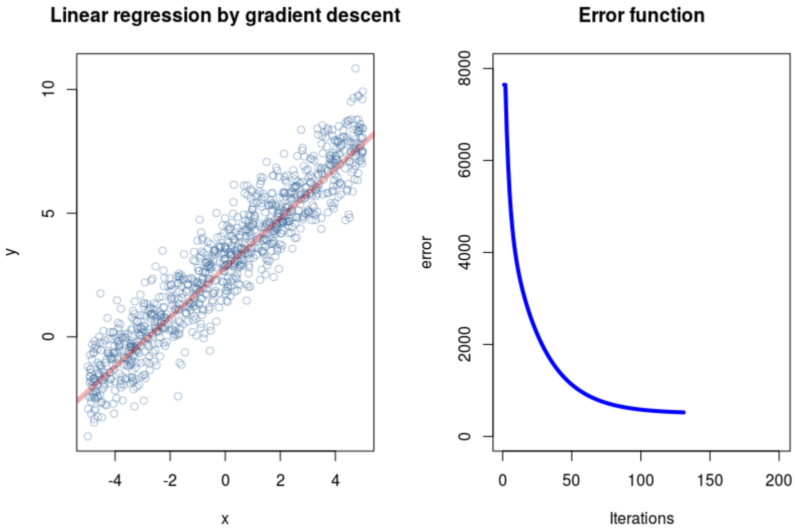

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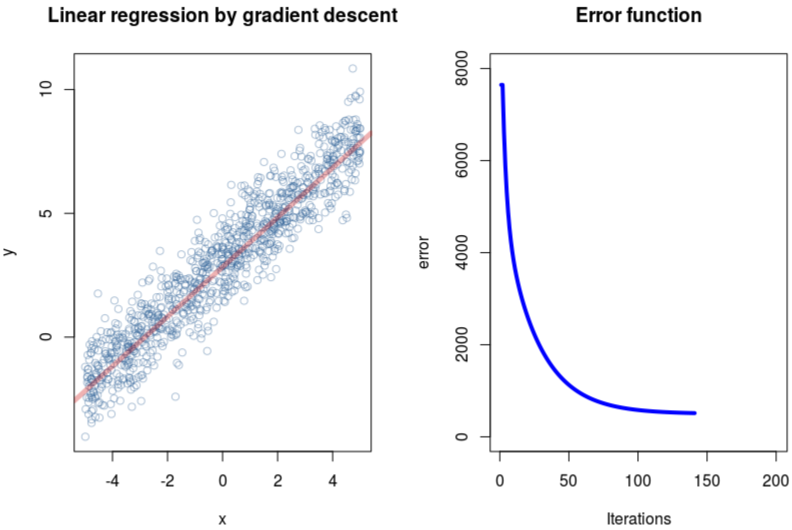

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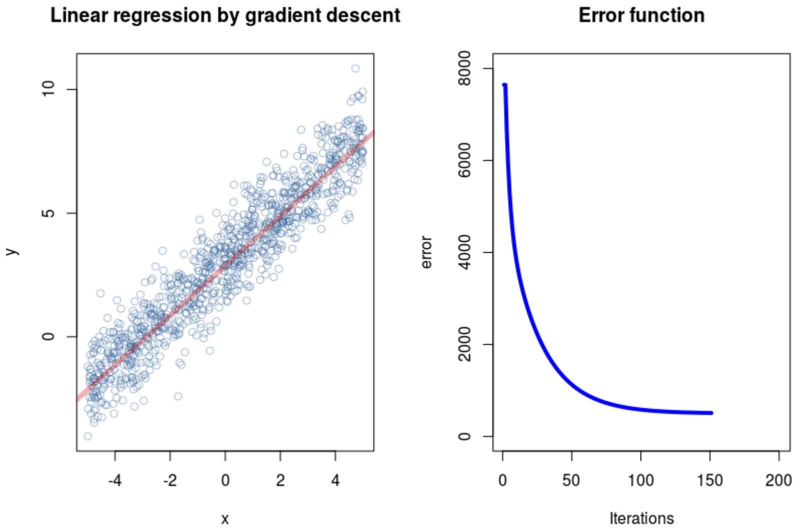

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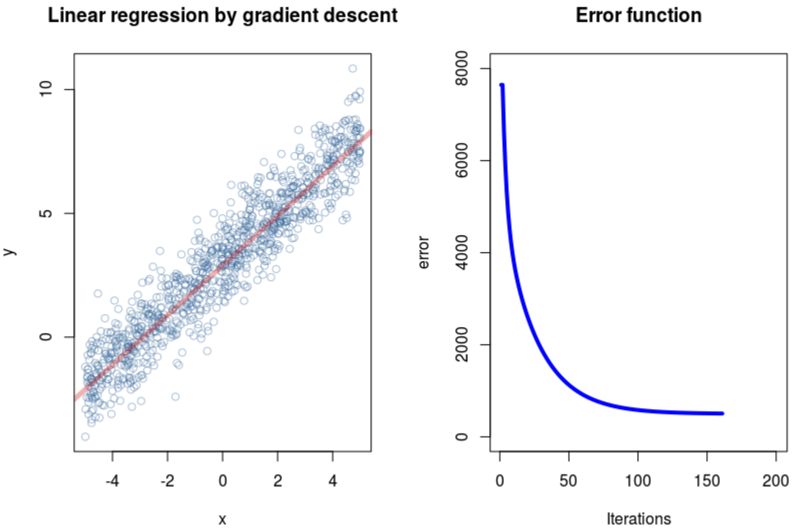

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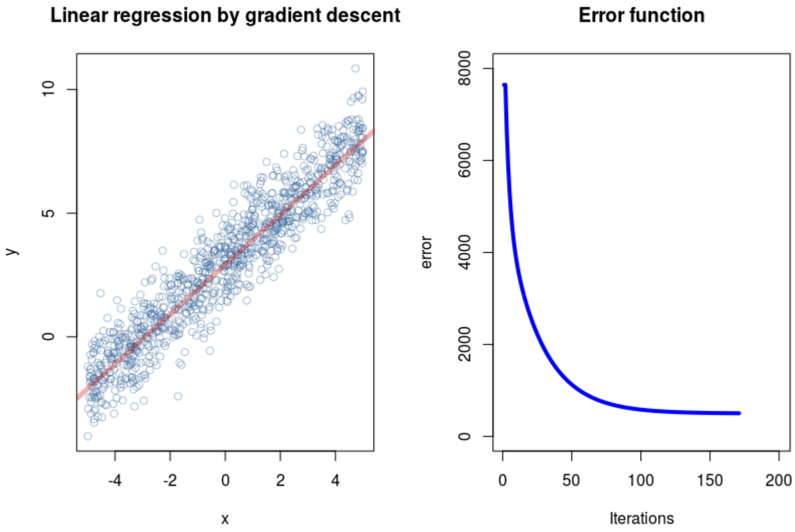

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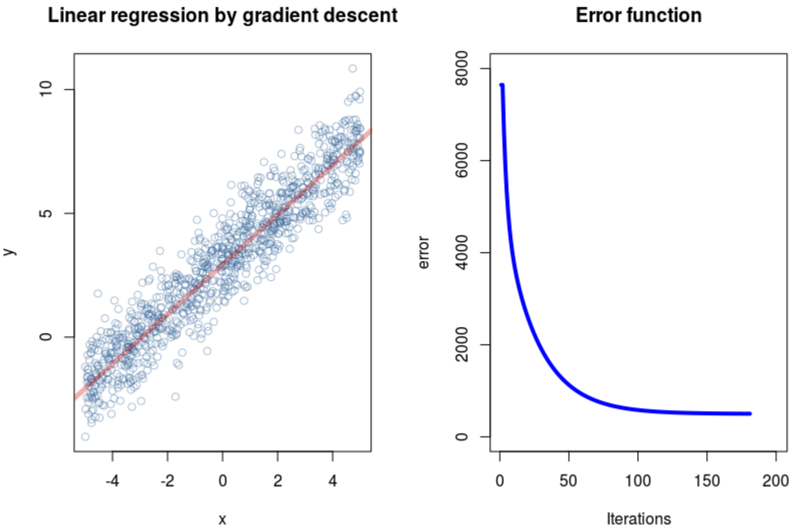

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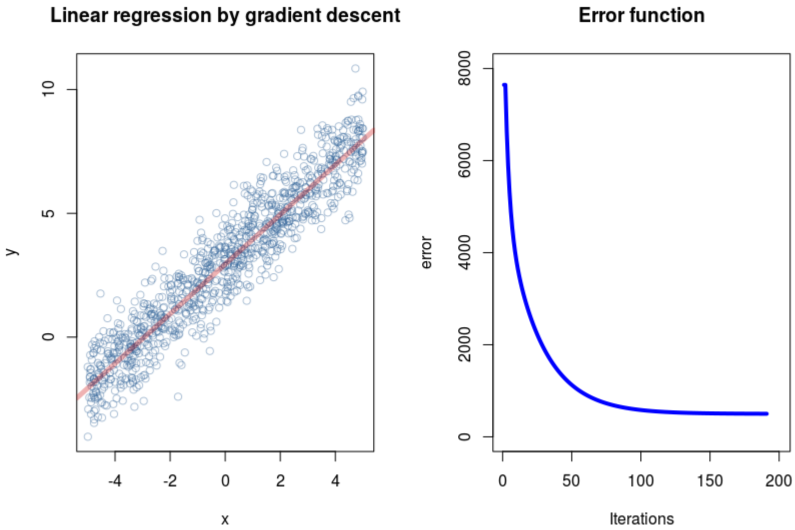

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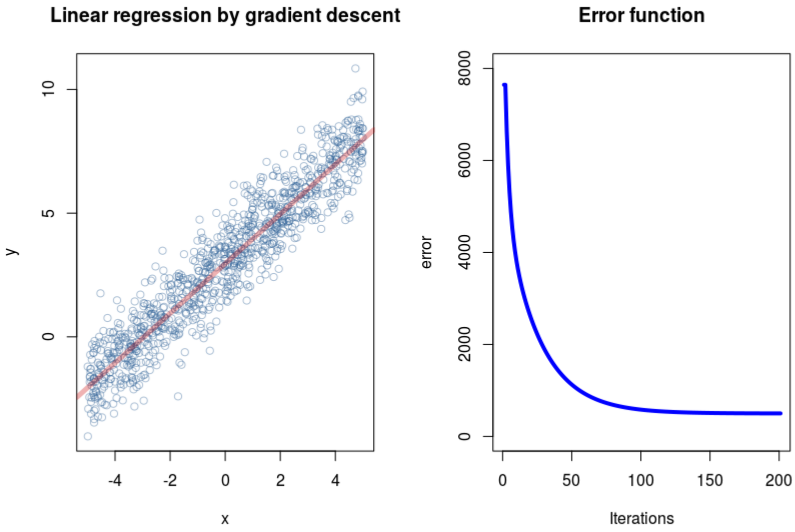

Finding the Minimum in Dimension One

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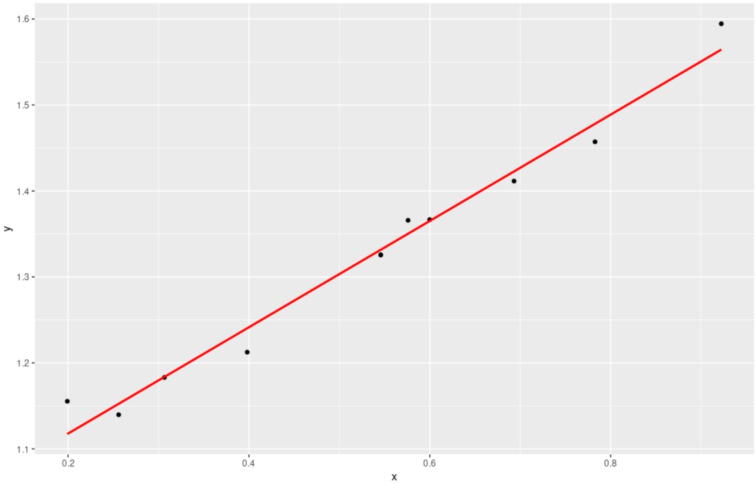
$$\frac{\partial E}{\partial w_1} = 0 \quad \Leftrightarrow \quad w_1 = \frac{\frac{1}{p}\sum_{k=1}^{p}(f_k - \bar{f})(x_k - \bar{x})}{\frac{1}{p}\sum_{k=1}^{p}(x_k - \bar{x})^2}$$

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

Effect of Outliers



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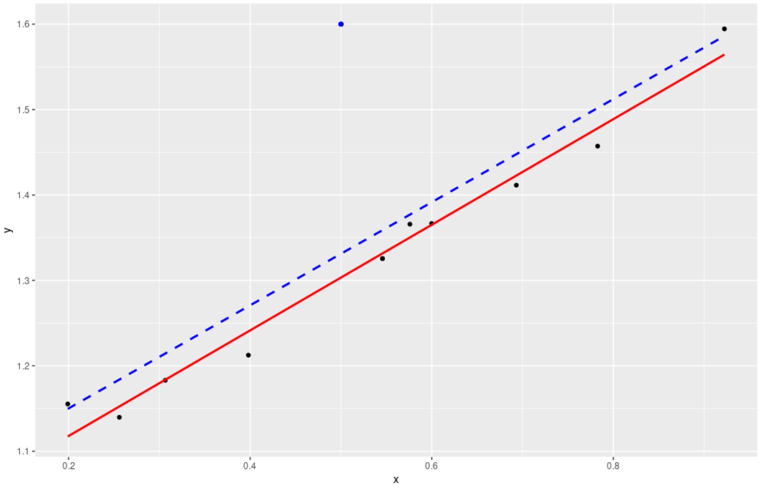

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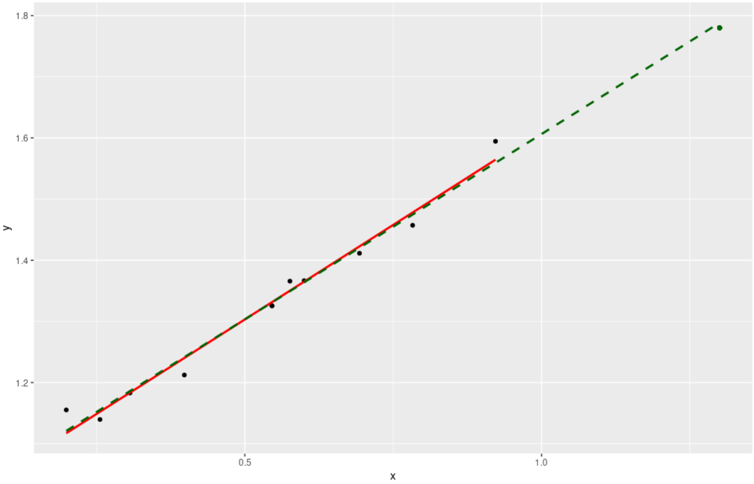

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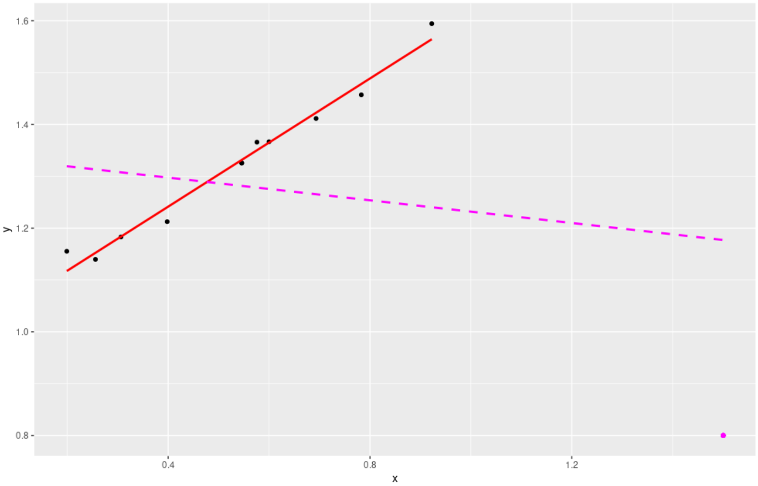

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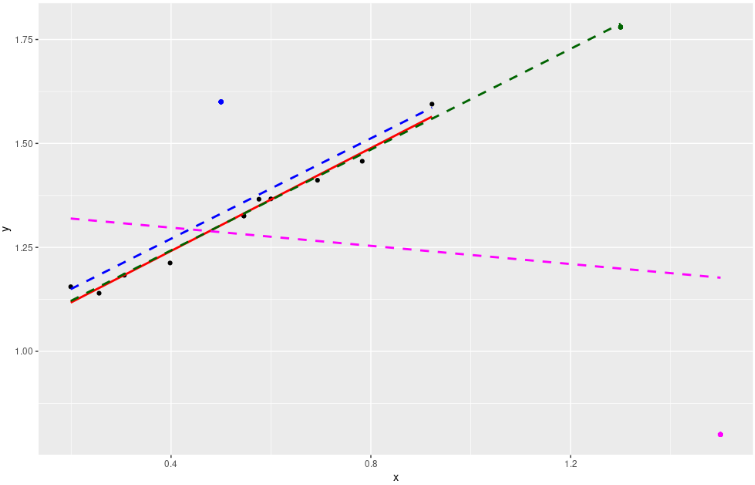
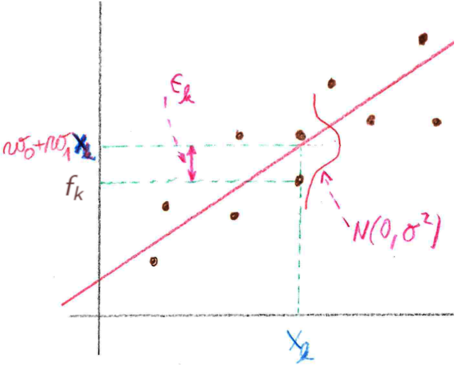


Maximum Likelihood vs Least Squares (Dim 1)

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 ϵ_k are independent, normally distributed noise values with mean 0 and some variance σ^2



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

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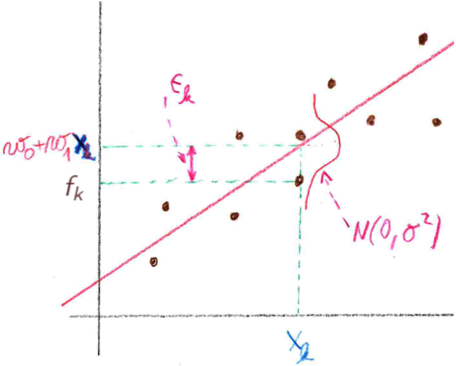

How "probable" is it to generate the correct $f_1, \ldots, f_p$?

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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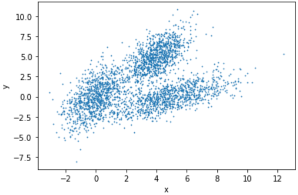
- Linear models are prone to outliers.

Unsupervised Learning

Clustering

Often data form clusters based on some notion of similarity.



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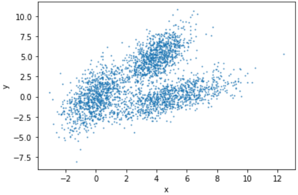

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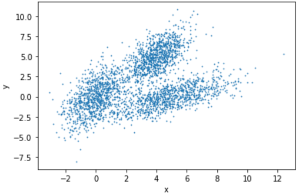
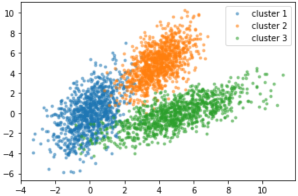


This means that the data distribution is *multimodal*, i.e., contains several regions of higher probability mass.

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

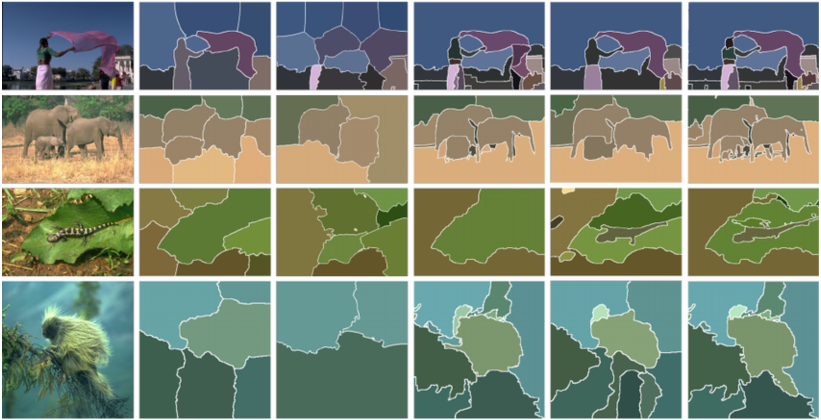


Motivation

Clustering is useful, e.g., in

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

Segmentation



Clustering Problem

Consider a dataset

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

Note that no target class/value is provided.

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

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For concreteness:

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

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

K-Means Clustering

K-means clustering

The K-means clustering model consists of

- The number of clusters K

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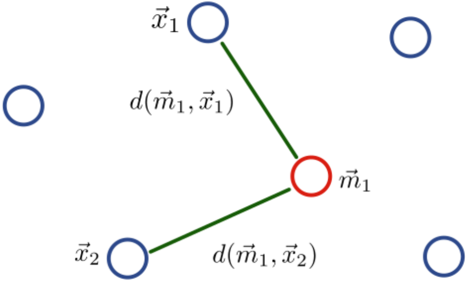
How good is a given model?

Error Function

Measure the distance of inputs $\vec{x}_i$ to their cluster prototypes $\vec{m}_j$



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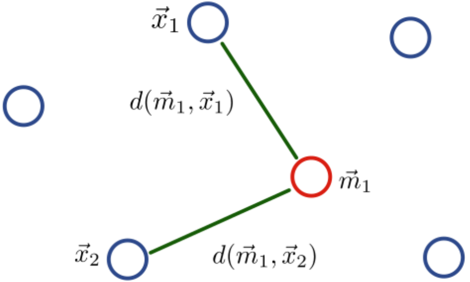

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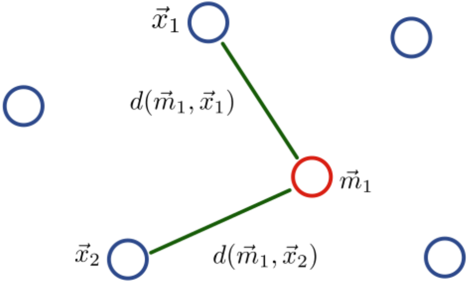

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We aim to *minimize* this error, i.e., to find proper positions of cluster prototypes and their assignment to minimize the total squared distance of examples to their prototypes.

K-means Clustering Complexity

The Problem K-means clustering problem (optimization):
Given a set $D = \{\vec{x}_1, \ldots, \vec{x}_p\}$ where $\vec{x}_k \in \mathbb{R}^n$ for all $k = 1, \ldots, p$ and an integer K, minimize

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

Theorem

The K-means clustering problem is NP-hard.

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

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

K-means Clustering Algorithm

The Problem: Minimize

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

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- If we fix $\{\vec{m}_j\}$, we can minimize $E(\{q_{ij}\}, \{\vec{m}_j\})$ by setting $q_{ij} = 1$ iff $\vec{m}_j$ is the *closest prototype* to $\vec{x}_i$.

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

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

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

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

K-Means Clustering Algorithm

Algorithm 1 K-means clustering

```
Initialize K cluster centers m_1, m_2, ..., m_K randomly
repeat
    for each data point x_i do
        Assign x_i to the nearest centroid, i.e., set q_ij = 1 for
            j = arg min_j d(x_i, m_j)^2
    end for
    for each cluster prototype m_j do
        Update m_j to be the centroid of all points assigned to it
            m_j = (1 / sum_{i=1}^{p} q_ij) sum_{i=1}^{p} q_ij x_i
    end for
until convergence
```

Initialize K cluster centers $\vec{m}_1, \vec{m}_2, \ldots, \vec{m}_K$ randomly

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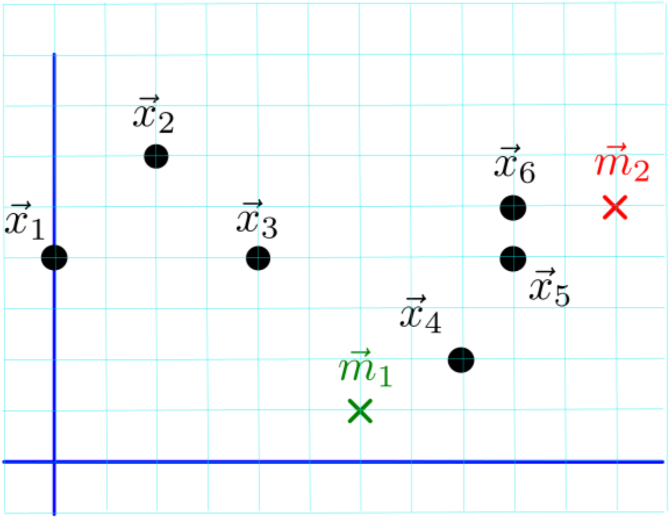
Example



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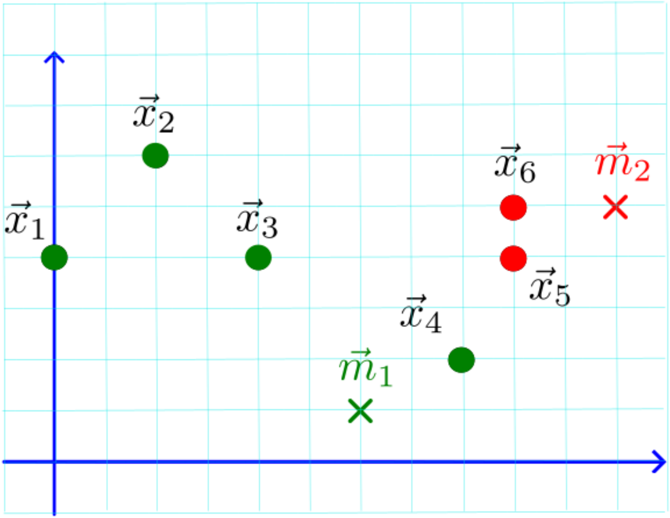

Lines 3-5: Assign examples to the prototypes.

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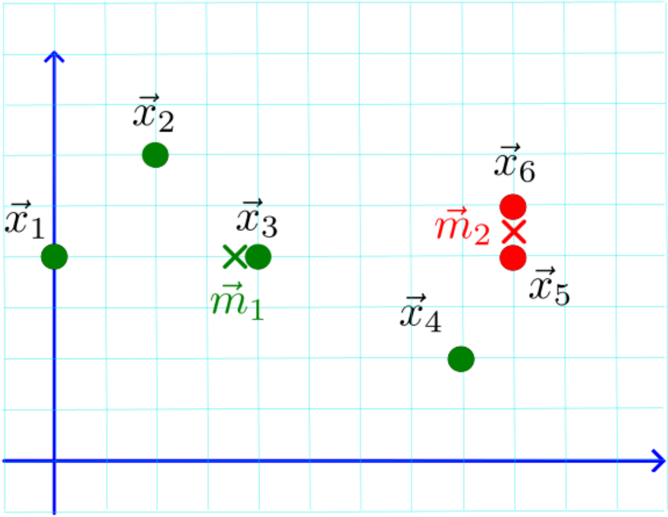

Lines 6-8: Move the prototypes to the centroids of their examples.

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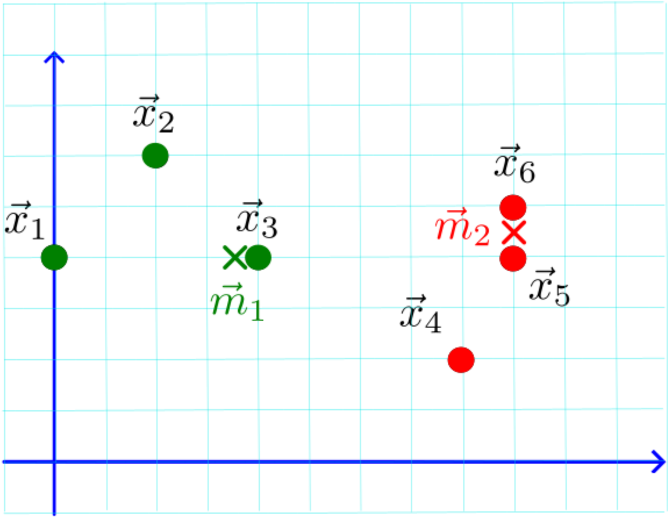

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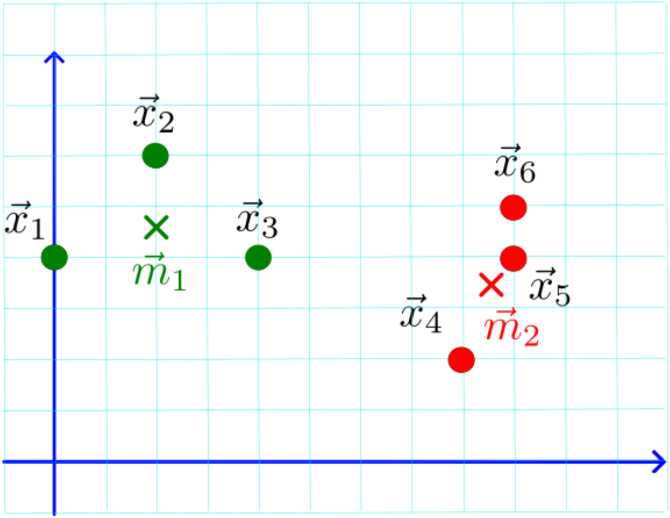

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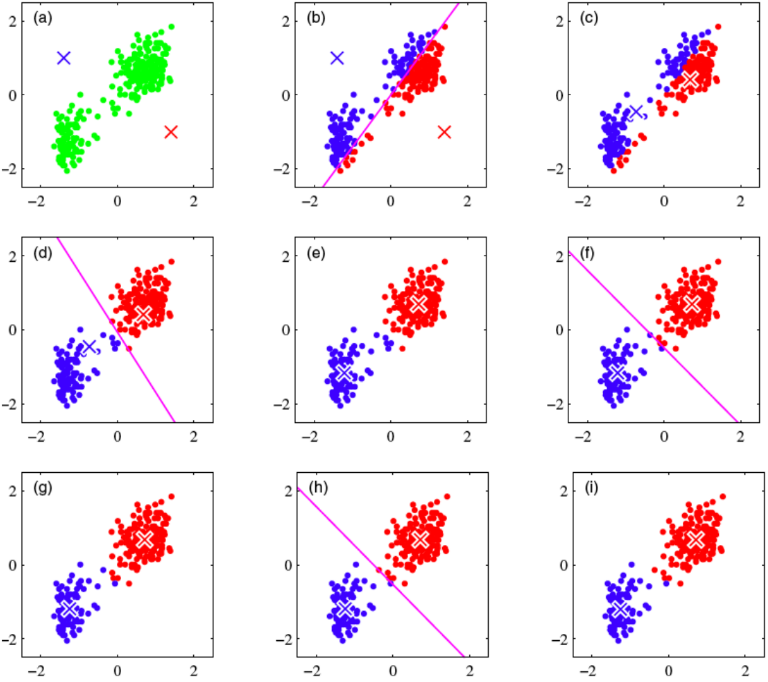
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
2
0
−2
−2
0
2

Convergence of K-means Clustering

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

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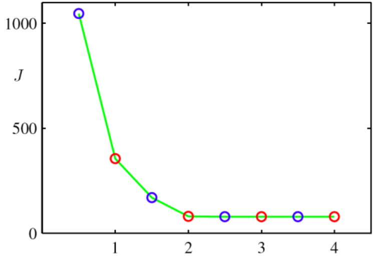
Example error development during training. Blue circles mean reassignment, and red circles mean moving prototypes.



Setting K - the Elbow Method

K-means clustering minimizes the *inertia* measure:

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

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

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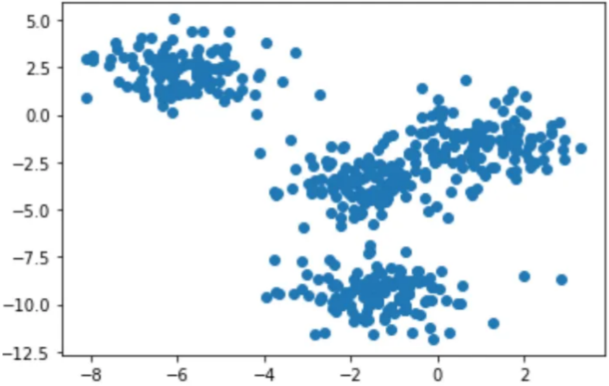
Note that the error does not consider the distance between the centers of the clusters.

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

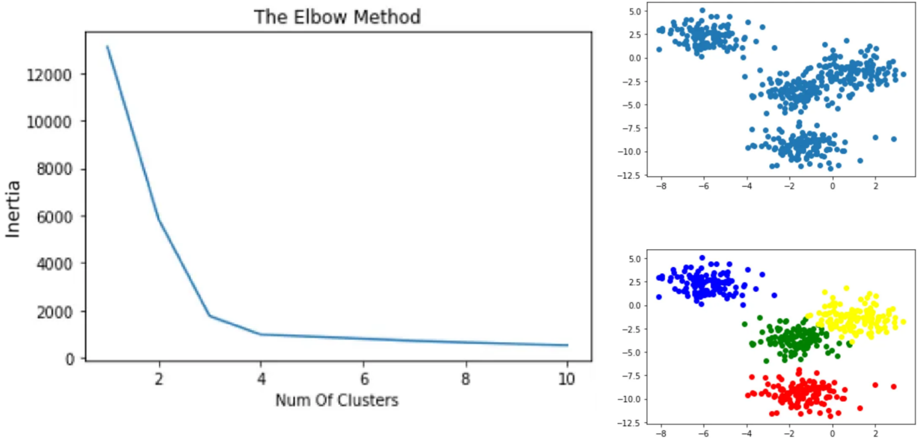
Elbow Method

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

Consider the following data:



Elbow Method



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

Bad Behavior

Minimizing $E(\{q_{ij}\}, \{\vec{m}_j\})$ starting from random positions of prototypes does not always produce “nice” results.

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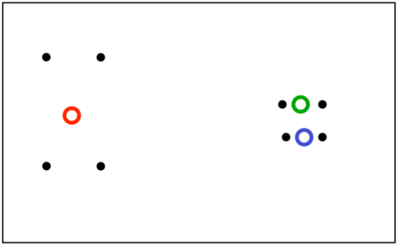
Some runs correspond to apparently bad solutions to the clustering problem even though a better solution exists.



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

Properties of K-means Clustering

- Prototype initialization is a big issue in K-means. There are various strategies. For example:
  - Start with all centers in a single corner.
  - Include randomness in the setting of centers throughout the algorithm.
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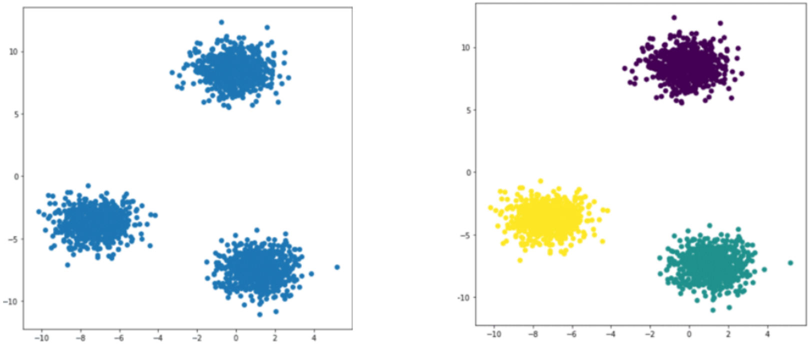
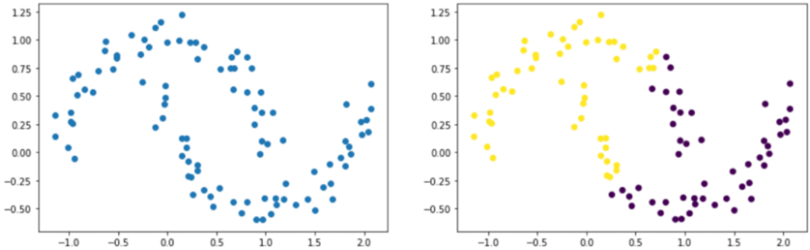
- As the squared error is behind the basic method, outliers may strongly affect its behavior (as in the linear regression case).
- Other problematic properties of data include
  - non-convex clusters
  - clusters of different sizes
  - non-linearly separable clusters
  - overlapping clusters


10
5
0
−5
−10
−10 −8 −6 −4 −2 0 2 4


1.25
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−1.0 −0.5 0.0 0.5 1.0 1.5 2.0

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

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

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More concretely:

- Maintain a set of clusters
- Initially, each $\vec{x}_i$ in its own cluster
- Repeat until only one cluster is left:
  - Pick two *closest clusters*
  - Merge them into a new cluster

Agglomerative Clustering

Consider a dataset

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

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

Idea:

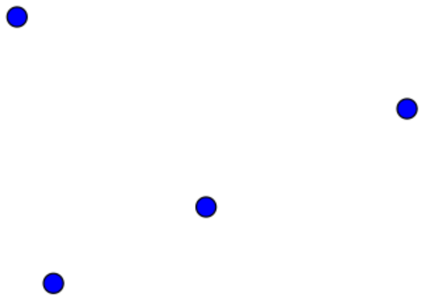
- Start by merging the closest examples (w.r.t. d)
- Incrementally build *larger clusters* by merging smaller clusters.

More concretely:

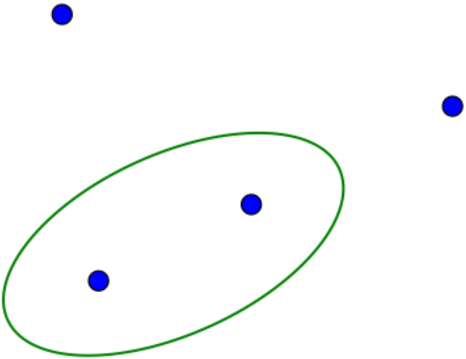
- Maintain a set of clusters
- Initially, each $\vec{x}_i$ in its own cluster
- Repeat until only one cluster is left:
  - Pick two *closest clusters*
  - Merge them into a new cluster

How do we determine the closest clusters?

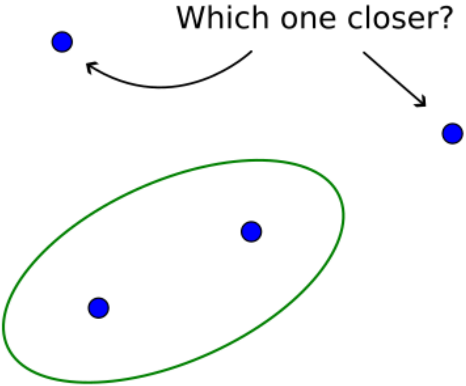
Closest Clusters



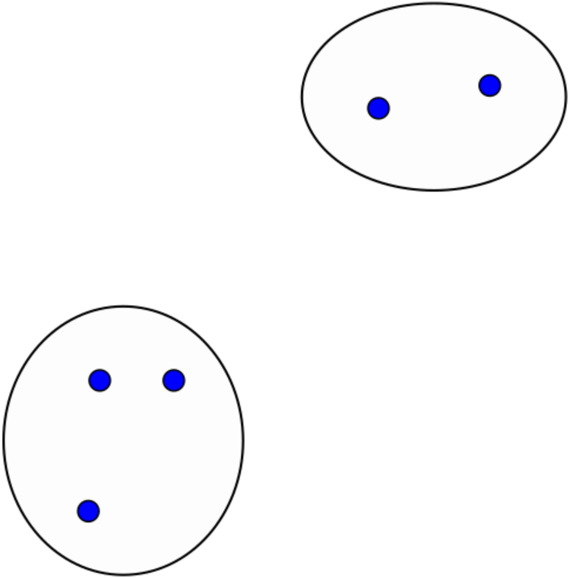
Closest Clusters



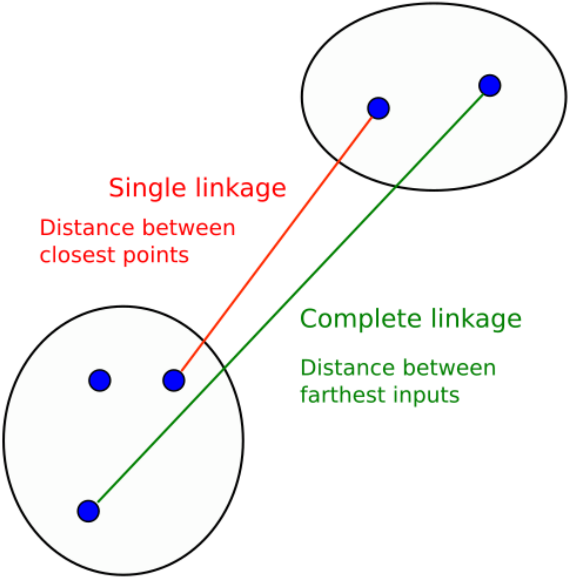
Closest Clusters



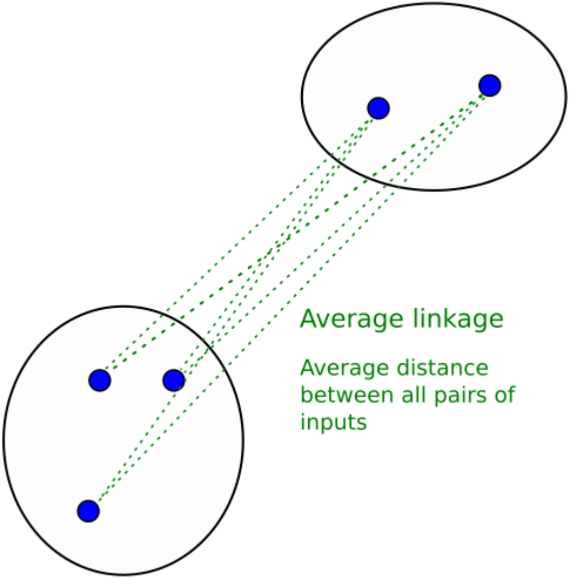
Distance Between Clusters



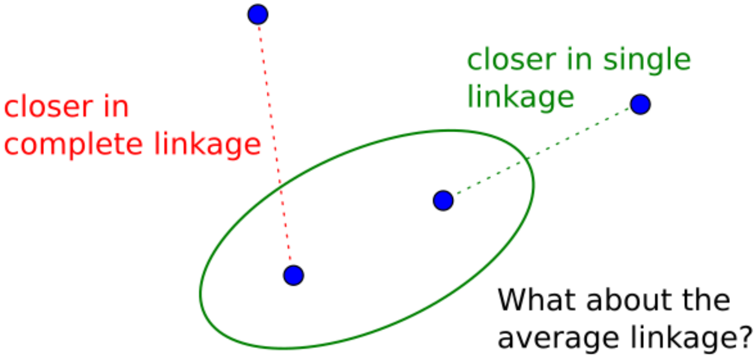
Distance Between Clusters



Distance Between Clusters

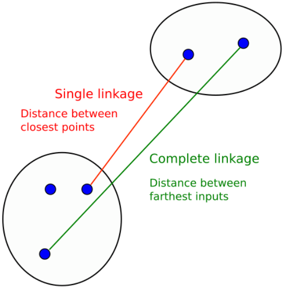


Which One is Closer?



Distance Between Clusters

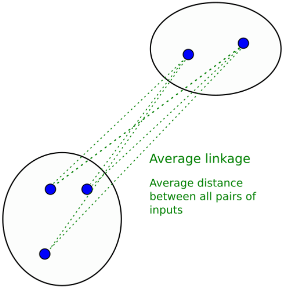
Consider two clusters $U_j, U_k \subseteq D$.



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

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

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

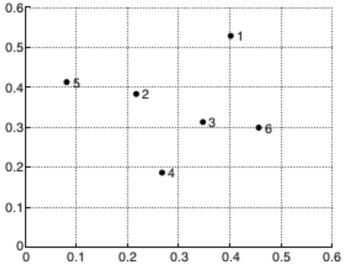


Each linkage can result in a different clustering.

Agglomerative Hierarchical Clustering Algorithm

Maintain a set of clusters
Initially, each $\vec{x}_i$ in its own cluster
repeat
    Pick two closest clusters
        Using the distance measure d and single, average, or complete linkage.
    Merge them into a new cluster
until only one cluster is left

Example

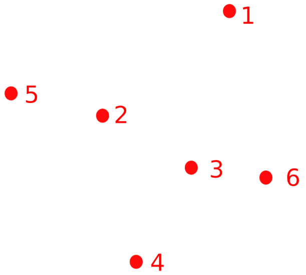


Point	x Coordinate	y Coordinate
p1	0.40	0.53
p2	0.22	0.38
p3	0.35	0.32
p4	0.26	0.19
p5	0.08	0.41
p6	0.45	0.30

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

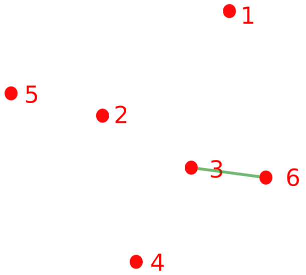
Example - Single Linkage

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



Example - Single Linkage

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

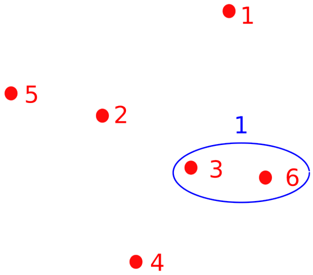


$$d(3,6) = 0.11$$

which is the minimum distance between points.

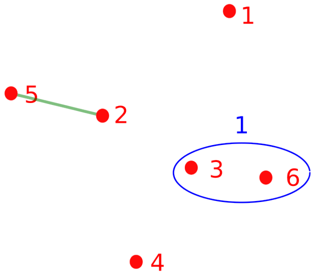
Example - Single Linkage

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



Example - Single Linkage

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

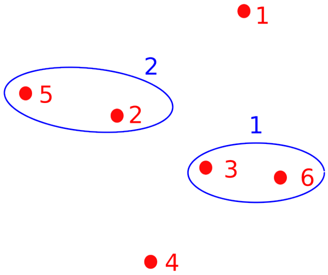


$$d(2,5) = 0.14$$

which is the second smallest distance.

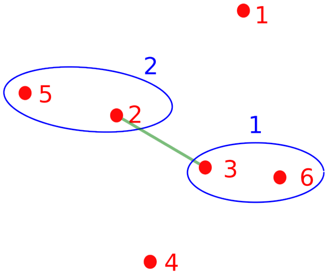
Example - Single Linkage

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



Example - Single Linkage

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

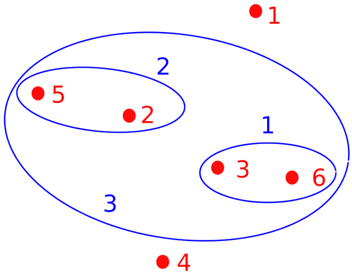


$$d(2,3) = 0.15 = \min\{d(2,3), d(2,6), d(5,3), d(5,6)\}$$

which is smaller than
$d(1,2) = 0.24$,
$d(1,3) = 0.22$,
$d(4,2) = 0.2$,
$d(4,3) = 0.16$,
$d(4,1) = 0.37$
the min. distances of points in all other pairs of clusters.

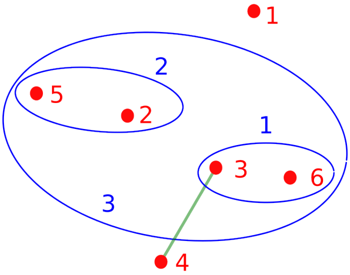
Example - Single Linkage

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



Example - Single Linkage

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

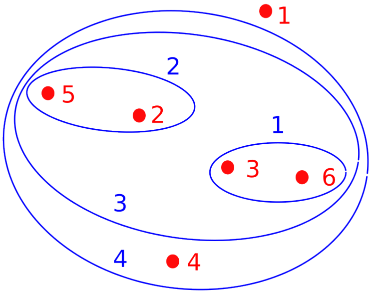


$$d(4,3) = 0.15$$
$$= \min\{d(4,3), d(4,5), d(4,2), d(4,6)\}$$

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

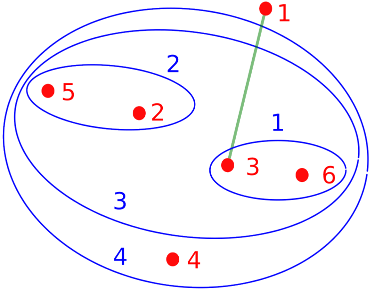
Example - Single Linkage

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



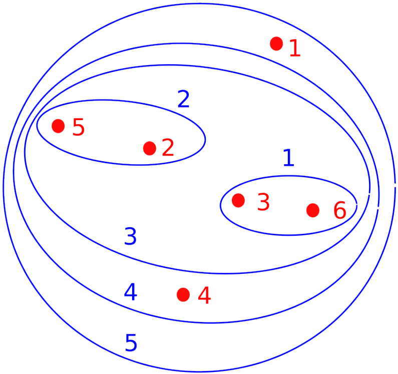
Example - Single Linkage

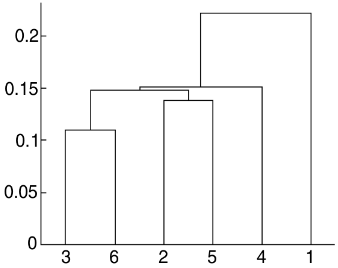
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



Example - Single Linkage

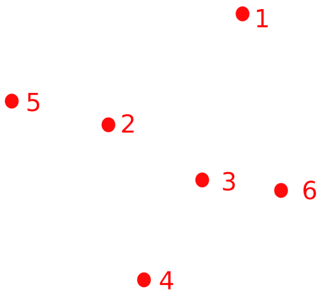
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00





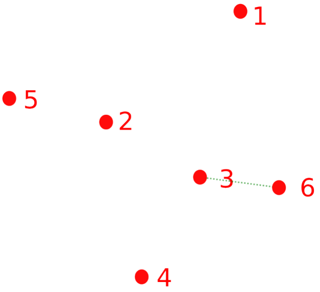
Example - Average Linkage

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



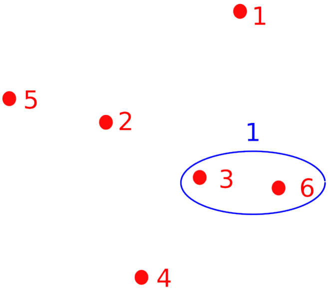
Example - Average Linkage

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



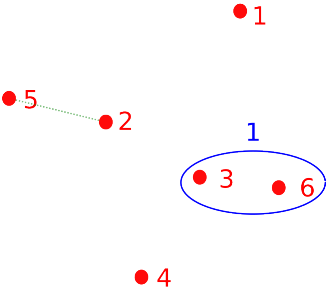
Example - Average Linkage

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



Example - Average Linkage

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

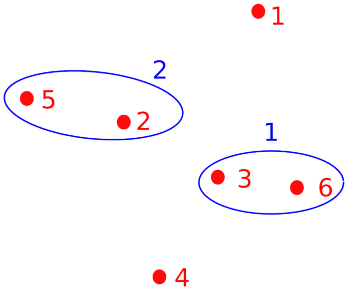


$$d(2,5) = 0.14$$

which is second smallest distance.

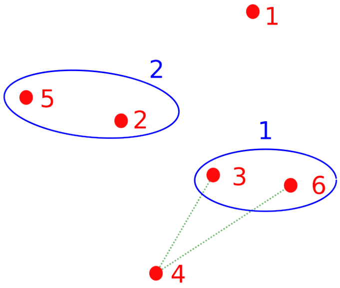
Example - Average Linkage

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



Example - Average Linkage

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



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

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

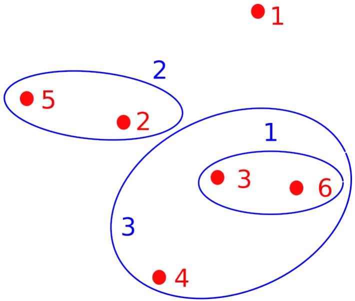
which is smaller than the average distance between all points of clusters $1, 2$:

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

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

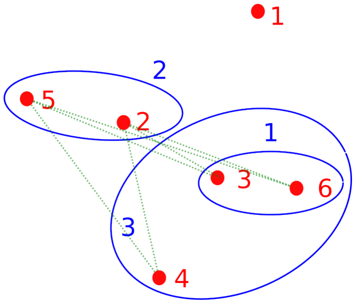
Example - Average Linkage

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



Example - Average Linkage

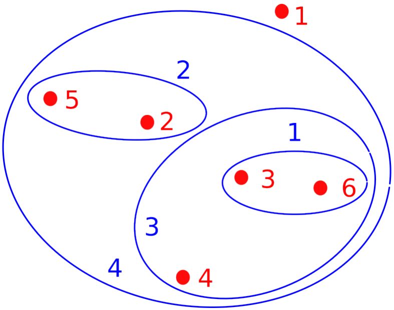
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



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

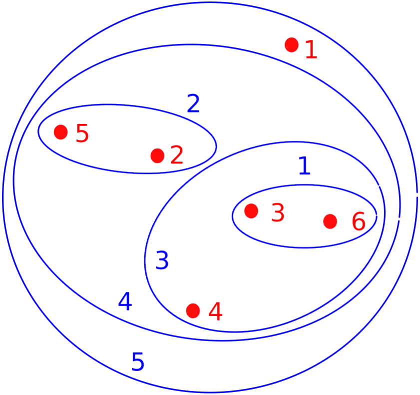
Example - Average Linkage

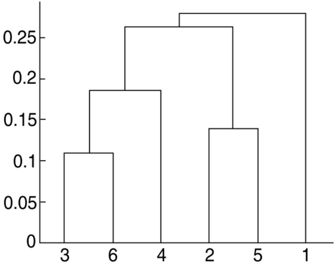
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00



Example - Average Linkage

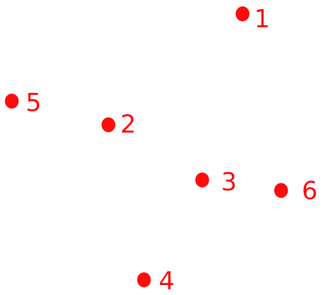
	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.16	0.28	0.11
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00





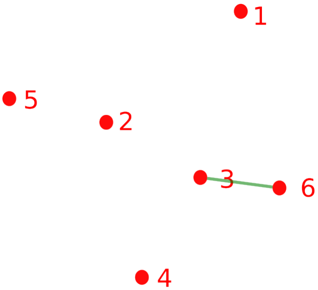
Example - Complete Linkage

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



Example - Complete Linkage

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

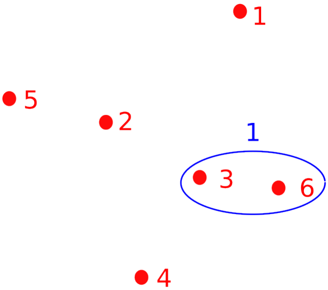


$$d(3,6) = 0.11$$

which is the minimum distance between points.

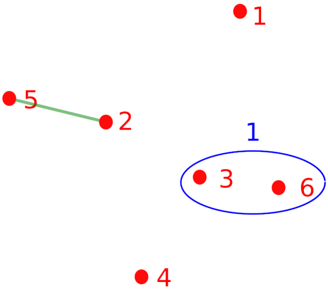
Example - Complete Linkage

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



Example - Complete Linkage

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

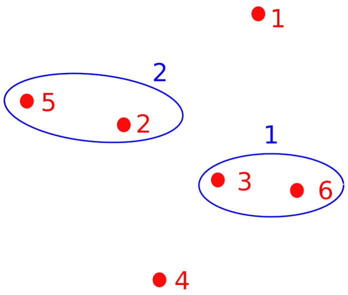


$$d(2,5) = 0.14$$

which is the second smallest distance.

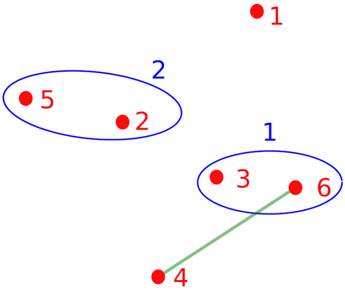
Example - Complete Linkage

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



Example - Complete Linkage

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

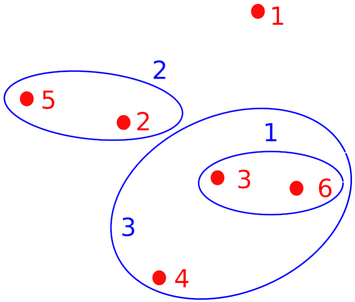


$$d(4,6) = 0.22 = \max\{d(4,3), d(4,6)\}$$

which is smaller than
$d(4,5) = 0.29$,
$d(1,5) = 0.34$,
$d(1,6) = 0.23$,
$d(5,6) = 0.39$,
$d(4,1) = 0.37$
the max distances of points in all other pairs of clusters.

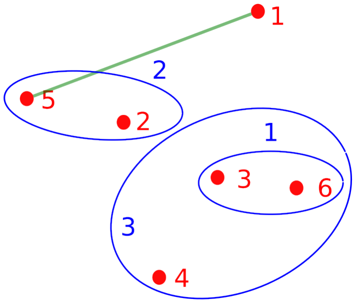
Example - Complete Linkage

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



Example - Complete Linkage

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

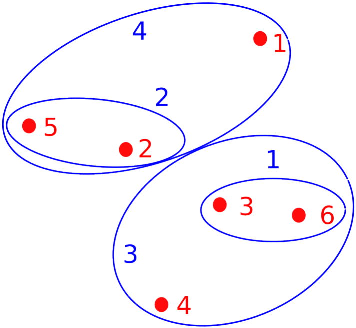


$$d(1,5) = 0.34$$

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

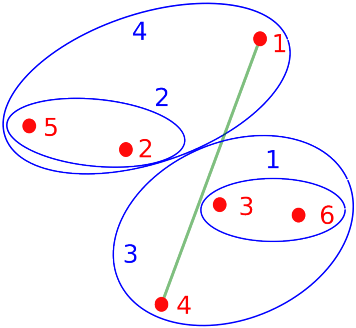
Example - Complete Linkage

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



Example - Complete Linkage

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



Example - Complete Linkage

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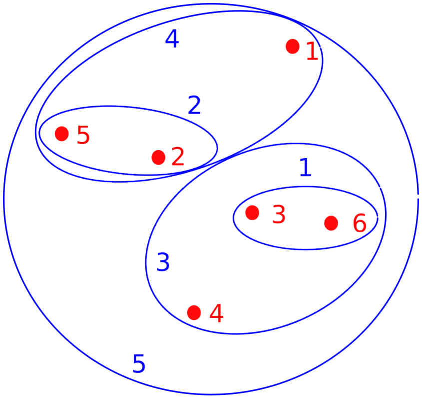
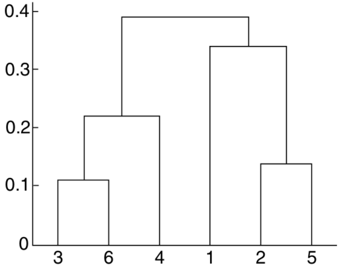
p4	0.37	0.20	0.16	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00





Properties of Agglomerative Hierarchical Clustering

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

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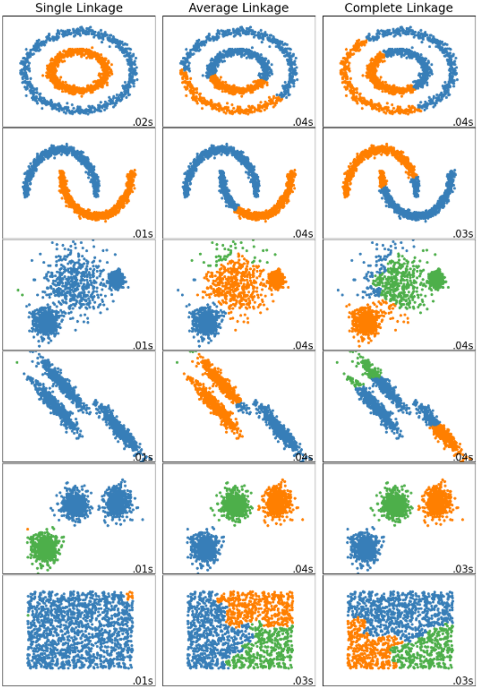
- Provides hierarchy of clusters - different cut levels provide different levels of coarseness of clusters
- Compared with k-means, it does not depend on the initialization and may provide better clusters than k-means.

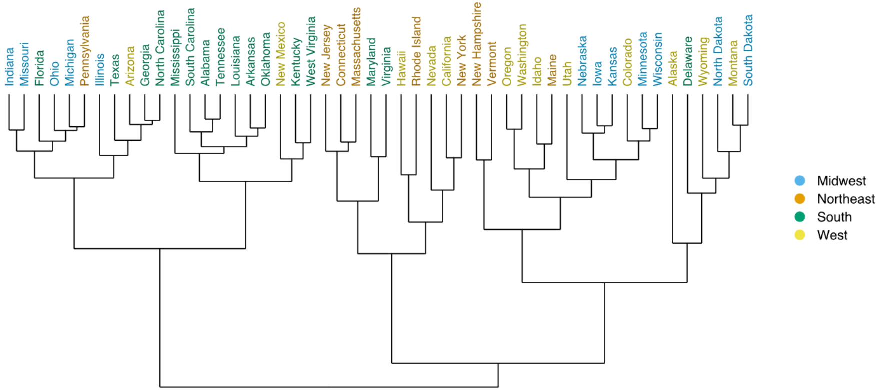
- Lack of global objective function
  - The agglomerative hierarchical clustering uses local criteria to decide which clusters to merge.
- Agglomerative clustering has a "rich get richer" behavior that leads to uneven cluster sizes
- Merging decision cannot be undone - bad for noisy data
- Computationally expensive.


Single Linkage
Average Linkage
Complete Linkage
.02s
.04s
.04s
.01s
.04s
.03s
.01s
.04s
.04s
.01s
.04s
.04s
.01s
.04s
.03s
.01s
.03s
.03s

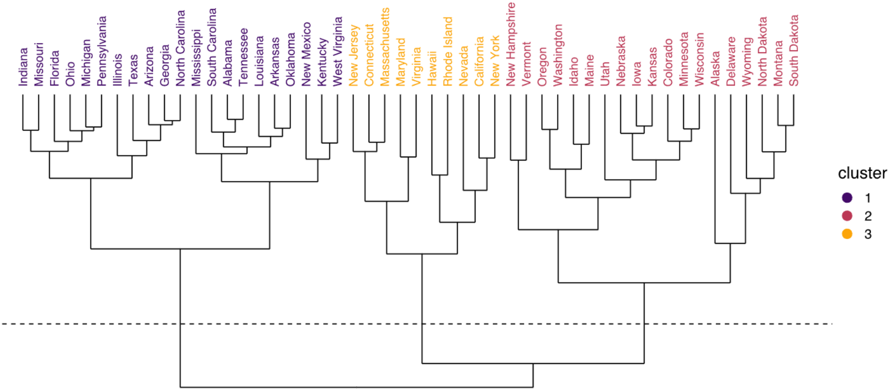
State level statistics for US

```
# A tibble: 50 × 20
   state      homeo…¹ multi…² income med_i…³ poverty fed_s…⁴ smoke murder robbery
   <chr>        <dbl>   <dbl>  <dbl>   <dbl>   <dbl>   <dbl> <dbl>  <dbl>   <dbl>
 1 Alabama       71.1    15.5  22984   42081    17.1   11.7   24.8    8.2   141. 
 2 Alaska        64.7    24.6  30726   66521     9.5   16.8   25      4.8    80.9
 3 Arizona       67.4    20.7  25680   50448    15.3    9.85  20.4    7.5   144. 
 4 Arkansas      67.7    15.2  21274   39267    18      9.61  23.5    6.7    91.1
 5 Californ…     57.4    30.7  29188   60883    13.7    8.89  15.2    6.9   176. 
 6 Colorado      67.6    25.6  30151   56456    12.2    9.15  19.9    3.7    84.6
 7 Connecti…     69.2    34.6  36775   67740     9.2   14.8   16.5    2.9   113  
 8 Delaware      73.6    17.7  29007   57599    11      8.89  20.7    4.4   155. 
 9 Florida       69.7    30    26551   47661    13.8    9.62  21.6    5     169. 
10 Georgia       67.2    20.5  25134   49347    15.7    8.88  22.2    6.2   155. 
# … with 40 more rows, 10 more variables: agg_assault <dbl>, larceny <dbl>,
#   motor_theft <dbl>, soc_sec <dbl>, nuclear <dbl>, coal <dbl>,
#   tr_deaths <dbl>, tr_deaths_no_alc <dbl>, unempl <dbl>, popdens2010 <dbl>,
#   and abbreviated variable names ¹homeownership, ²multiunit, ³med_income,
#   ⁴fed_spend
```

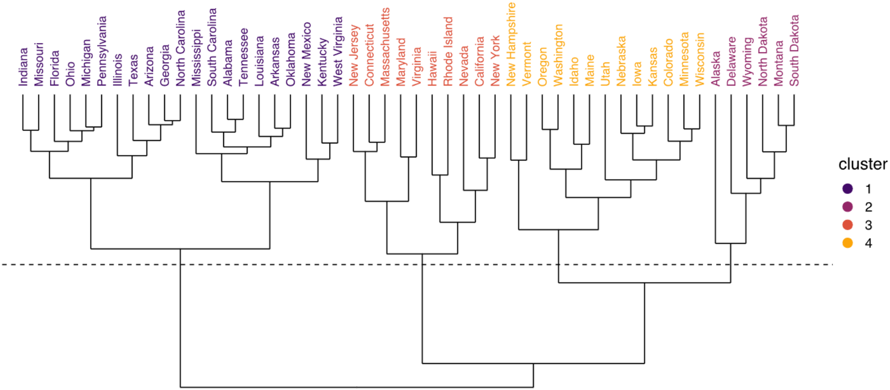
State level statistics for US



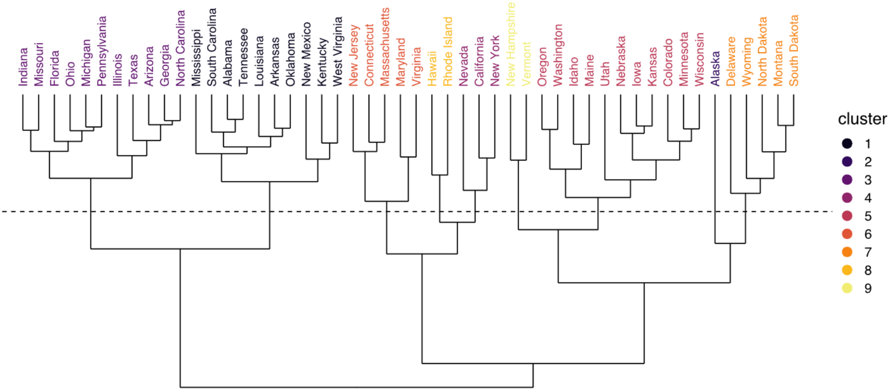
State level statistics for US



State level statistics for US



State level statistics for US



Cluster Validation

Cluster Validity

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

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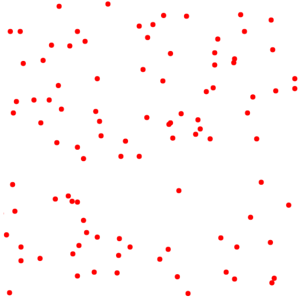
For cluster analysis (=unsupervised learning), the analogous question is:

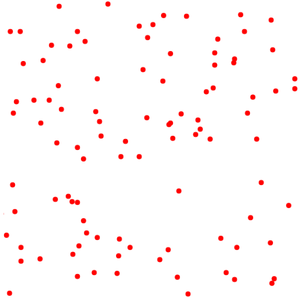
How to evaluate the “goodness” of the resulting clusters?

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

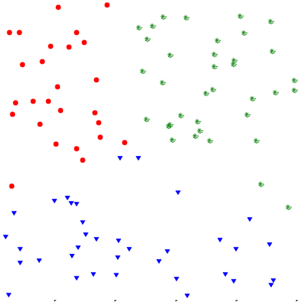
Random points:



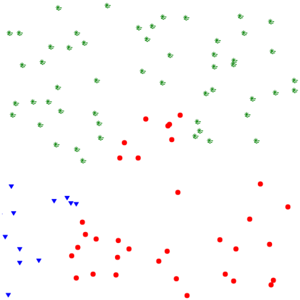
Random points:



K-means



Hierarchical



Different Aspects of Cluster Validation

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

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3. External Validation: Compare the cluster analysis results to externally known class labels (class labels).
4. Compare clusterings to determine which is better.
5. Determining the '**correct**' number of clusters.

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

Measures of Cluster Validity

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

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

Internal Index

Consider a dataset

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

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

No other information has been provided.

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

Internal Index

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

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

No other information has been provided.

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

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

For concreteness:

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

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

Cohesion and Separation

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

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

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$$\mathit{proximity}(\vec{x}, \vec{z})$$

The proximity might be, e.g.,

- the distance $d(\vec{x}, \vec{z})$,
- the square of the distance, that is $d(\vec{x}, \vec{z})^2$,
- any other notion of dissimilarity based on the application.

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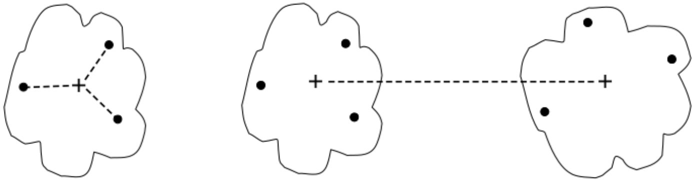
- the square of the distance, that is $d(\vec{x}, \vec{z})^2$,
- any other notion of dissimilarity based on the application.

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

Prototype-based Cohesion and Separation



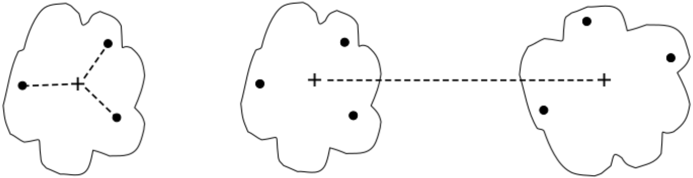
Prototype-based cohesion = the similarity of examples within a given cluster to a prototype of the cluster (e.g., centroid).

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

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

Note that the prototype **does not** have to be an element of U_j.
Intuitively, cohesion is the proximity of cluster's examples and a point somewhere "between" all examples of the cluster.

Prototype-based Cohesion and Separation



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

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

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

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

Prototype-based Cohesion and Separation

Summarize the prototype-based cohesion and separation as follows:

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

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$$\text{separation}(\mathcal{U}) = \sum_{j=1}^{K} |U_j| \mathit{separation}(U_j)$$
$$= \sum_{j=1}^{K} |U_j| \mathit{proximity}(\vec{m}_j, \vec{m})$$

If $\mathit{proximity}(\vec{x}, \vec{z})$ is defined as $d(\vec{x}, \vec{z})^2$ then the cohesion is the inertia.

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

Prototype-based Cohesion and Separation

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

Consider $\mathit{proximity}(\vec{x}, \vec{z}) = d(\vec{x}, \vec{z})^2$ and all prototypes to be centroids.

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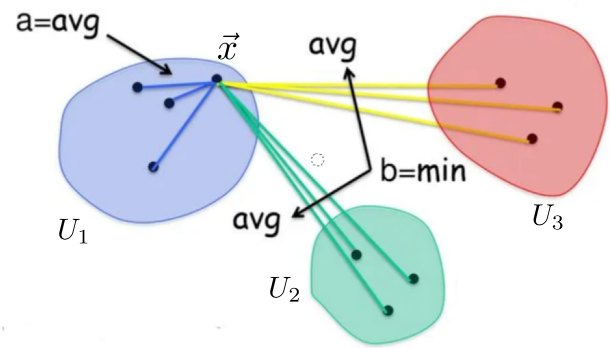
The following holds:

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

Note that TSS is determined by D.

Silouette Score

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



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

Silhouette Score

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

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$$a(\vec{x}) = \frac{1}{|U_j| - 1} \sum_{\vec{z} \in U_j \setminus \{\vec{x}\}} d(\vec{x}, \vec{z})$$

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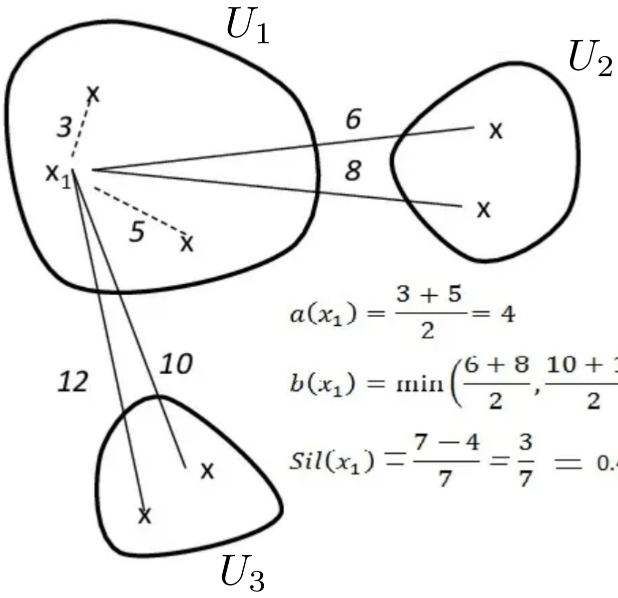
If $|U_j| > 1$ we define

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

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

Example

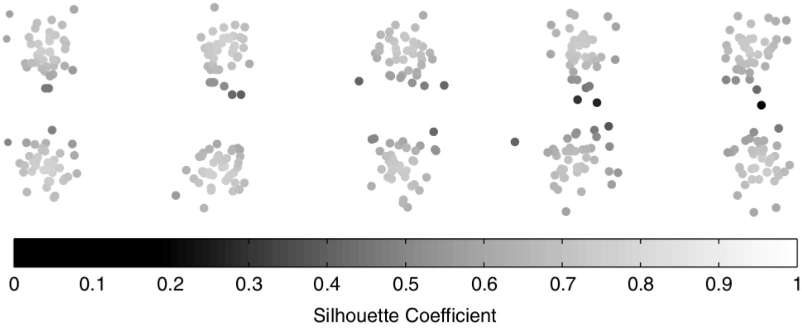


$$a(x_1) = \frac{3+5}{2} = 4$$

$$b(x_1) = \min\left(\frac{6+8}{2}, \frac{10+12}{2}\right) = 7$$

$$Sil(x_1) = \frac{7-4}{7} = \frac{3}{7} = 0.42$$

Example



Silhouette for Clusters and Clusterings

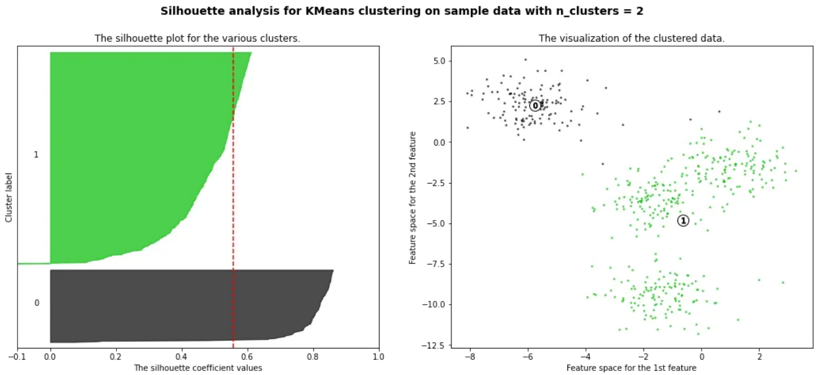
We have defined the silhouette for a single $\vec{x} \in D$.

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

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

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

Example



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

The red vertical line denotes the silhouette score for the whole dataset.

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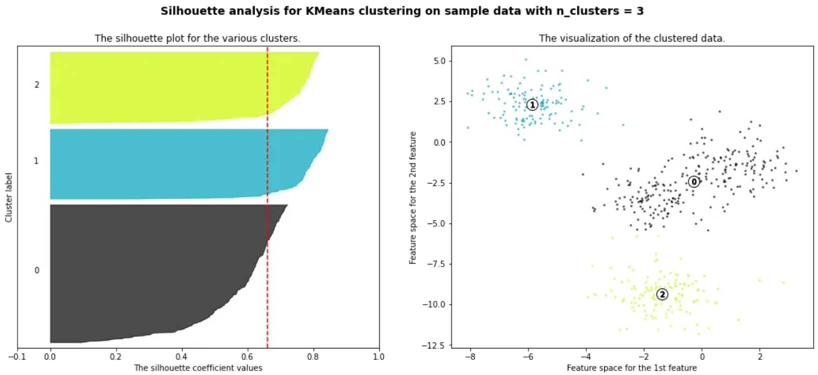

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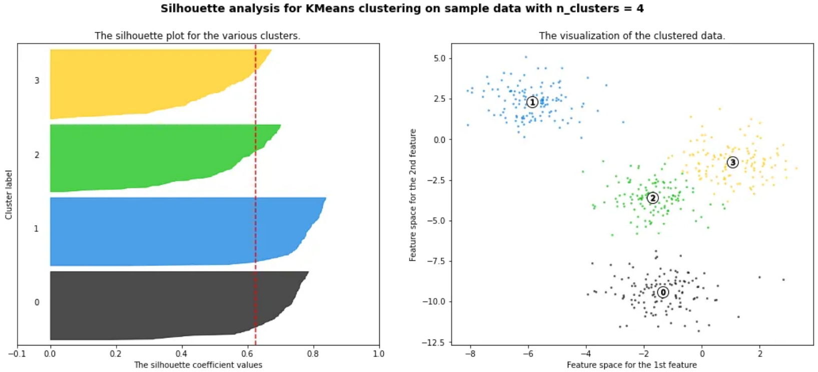

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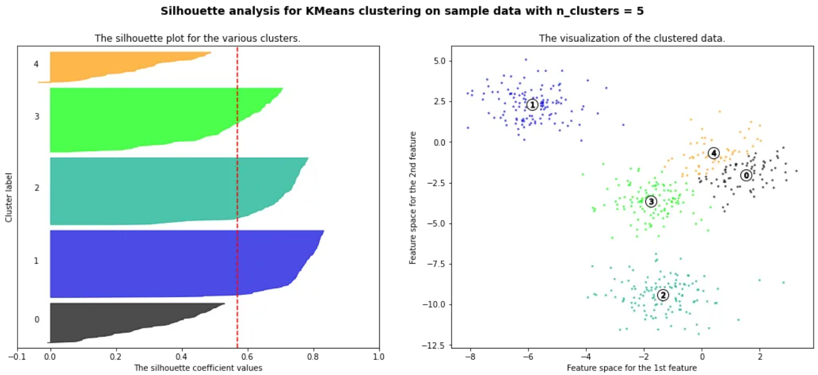

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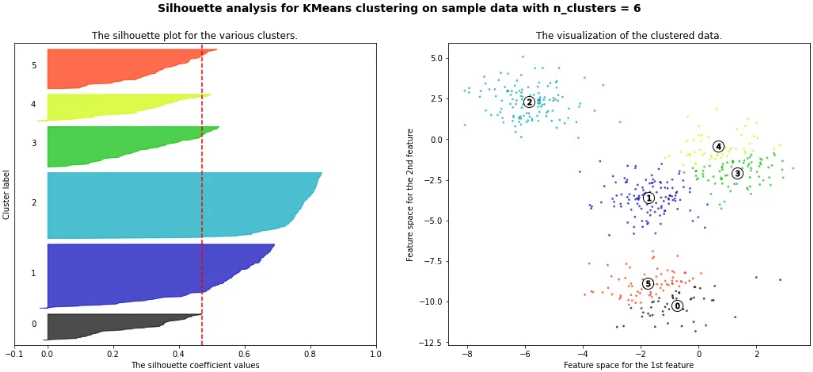

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External Index

Consider a *supervised learning* dataset

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

Here $c_i \in C$ is a class of $\vec{x}_i$.

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

We measure how the clustering conforms with the given classes.

Purity

Consider the clustering to be a classification model.

Define a classifier $h : D \to C$ such that given $\vec{x}_i \in U_j \in \mathcal{U}$

$$h(\vec{x}_i) = \text{the most frequent class in } U_j$$

Now we can measure the Accuracy of h.

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Accuracy of h is called *purity*.

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Is it a good measure?

Probably not; many clusters lead to high purity (each element in its own cluster means purity $= 1$).

Classifier Point of View

Given $\vec{x}_i$, denote by $\mathcal{U}(\vec{x}_i)$ the cluster $U_j \in \mathcal{U}$ containing $\vec{x}_i$.

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Distinguish the following types of *pairs* of examples:

- TP = number of examples of the same class and the same cluster

$$\text{TP} = |\{(i,j) \mid \mathcal{U}(\vec{x}_i) = \mathcal{U}(\vec{x}_j) \wedge c_i = c_j)\}$$

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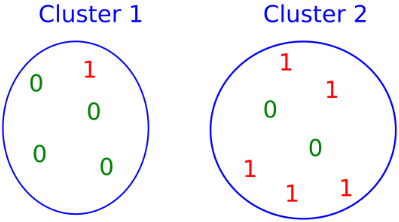
Now, we may apply all the measures from the supervised model.

Example



$$\text{TP} = \binom{4}{2} + \binom{5}{2} + \binom{2}{2}$$
$$= 6 + 10 + 1 = 17$$

$$\text{TN} = 4 * 5 + 1 * 2 = 22$$

$$\text{FP} = 1 * 4 + 5 * 2 = 14$$

$$\text{FN} = 1 * 5 + 4 * 2 = 13$$

		Cluster	
		same	*diff*
Class	*same*	TP=17	FN=13
	diff	FP=14	TN=22

Rand Index

Accuracy (in this area known as *Rand index*) is

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Note that the Rand index can be used to compare two clusterings: Simply consider class labels to be indicators of clusters.

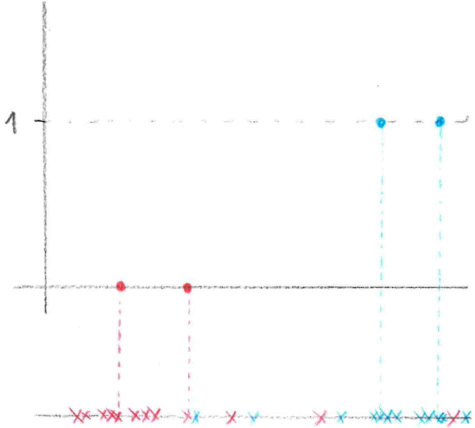
Similarly, we may compute the other measures such as Precision, Recall, and F_1 with all their benefits and limitations.

Logistic Regression

What about classification using regression?

Binary classification: Desired outputs 0 and 1

... we want to capture the probability distribution of the classes



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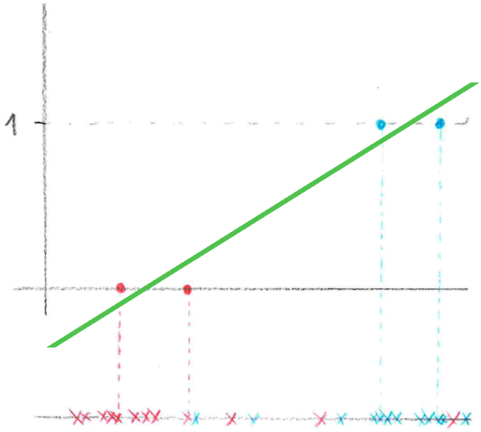

... does not capture the probability well (it is not probability at all)

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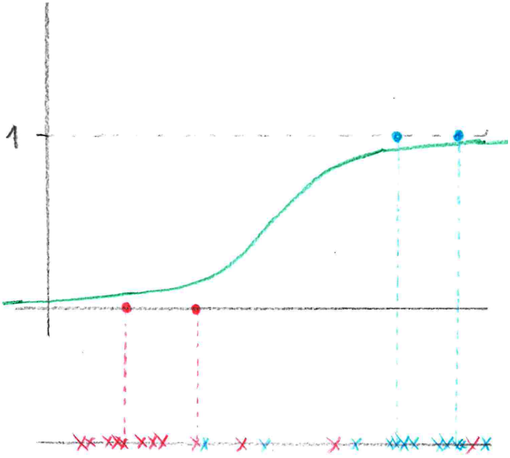

... logistic sigmoid $\frac{1}{1+e^{-(\vec{w}\cdot\tilde{\mathbf{x}})}}$ is much better!

Logistic Regression

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

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

Given $\vec{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$,

$$h[\vec{w}](\vec{x}) := \frac{1}{1 + e^{-\left(w_0 + \sum_{k=1}^{n} w_k x_k\right)}} = \frac{1}{1 + e^{-\vec{w}\cdot\tilde{\mathbf{x}}}}$$

Here

$$\tilde{\mathbf{x}} = (x_0, x_1, \ldots, x_n) \quad \text{where } x_0 = 1$$

is the *augmented feature vector*.

But what is the meaning of the sigmoid?

The model gives probability $h[\vec{w}](\vec{x})$ of the class 1 given an input $\vec{x}$.
But why do we model such probability using $1/(1+e^{-\vec{w}\cdot\tilde{\mathbf{x}}})$??

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Denote by $\bar{h}$ the probability $P(Y = 1 \mid X = \vec{x})$, i.e., the "true" probability of the class 1 given features $\vec{x}$.

The probability $\bar{h}$ cannot be easily modeled using a linear function (the probabilities are between 0 and 1).

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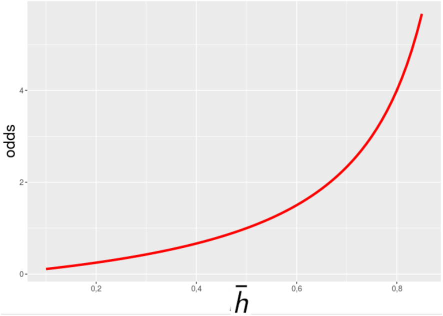
What about odds of the class 1?

$$odds(\bar{h}) = \bar{h}/(1 - \bar{h})$$



Better, at least it is unbounded on one side ...

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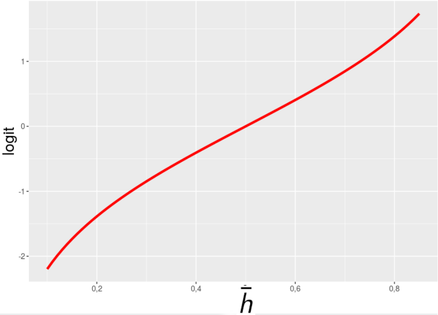
What about log odds (aka logit) of the class 1?

$$logit(\bar{h}) = \log(\bar{h}/(1 - \bar{h}))$$



Looks almost linear, at least for probabilities not too close to 0 or 1 ...

But what is the meaning of the sigmoid?

Assume that $\bar{h}$ is the actual probability of the class 1 for an "object" with features $\vec{x} \in \mathbb{R}^n$. Put

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and

$$\bar{h} = \frac{1}{1+e^{-\vec{w} \cdot \tilde{\mathbf{x}}}} = h[\vec{w}](\vec{x})$$

If we model log odds using a linear function, the probability is obtained by applying the logistic sigmoid on the result of the linear function.

Logistic Regression

- Given a set D of training samples:

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

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 $h[\vec{w}](\vec{x}_k) = 1 \,/\, \left(1 + e^{-\vec{w}\cdot\tilde{\mathbf{x}}_k}\right)$ where
$\tilde{\mathbf{x}}_k = (x_{k0}, x_{k1} \ldots, x_{kn})$, here $x_{k0} = 1$

Our goal: Find $\vec{w}$ such that for every $k = 1, \ldots, p$ we have that $h[\vec{w}](\vec{x}_k) \approx c_k$

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Recall that $h[\vec{w}](\vec{x}_k) = 1 \,/\, \left(1 + e^{-\vec{w}\cdot\tilde{\mathbf{x}}_k}\right)$ where
$\tilde{\mathbf{x}}_k = (x_{k0}, x_{k1} \ldots, x_{kn})$, here $x_{k0} = 1$

Our goal: Find $\vec{w}$ such that for every $k = 1, \ldots, p$ we have that $h[\vec{w}](\vec{x}_k) \approx c_k$

- **Binary Cross-entropy:**

$$E(\vec{w}) = -\sum_{k=1}^{p} c_k \log(h[\vec{w}](\vec{x}_k)) \;+\; (1 - c_k) \log(1 - h[\vec{w}](\vec{x}_k))$$

Gradient of the Error Function

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

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

Fact 1

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

This follows from the fact that E is convex.

Using the squared error with the logistic sigmoid would lead to a non-convex error with several minima!

Logistic Regression – Learning

Gradient Descent:

- Weights $\vec{w}^{(0)}$ are initialized randomly close to $\vec{0}$.

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

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

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\end{aligned}
$$

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

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

Proposition

For sufficiently small $\varepsilon > 0$, the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges (in a component-wise manner) to the global minimum of the error function E.

Logistic Regression - Using the Trained Model

We have already trained our logistic regression model, i.e., we have a vector of weights $\vec{w} = (w_0, w_1, \ldots, w_n)$.

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To decide whether a given $\vec{x}$ belongs to the class 1 we use $h[\vec{w}]$ as a Bayes classifier: Assign $\vec{x}$ to the class 1 iff $h[\vec{w}](\vec{x}) \geq 1/2$.

Other thresholds can also be used depending on the application and properties of the model. In such a case, given a threshold $\xi \in [0, 1]$, assign $\vec{x}$ to the class 1 iff $h[\vec{w}](\vec{x}) \geq \xi$.

Maximum Likelihood vs Cross-entropy (Dim 1)

Fix a training set $D = \{(x_1, c_1), (x_2, c_2), \ldots, (x_p, c_p)\}$

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and 0 otherwise.

Here w_0, w_1 are **unknown weights**.

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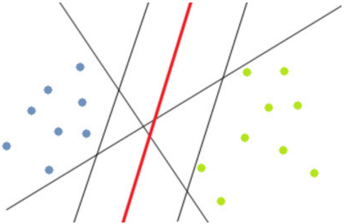
The following conditions are equivalent:

- w_0, w_1 minimize the binary cross-entropy E
- w_0, w_1 maximize the likelihood (i.e., the "probability") of generating the correct values $c_1, \ldots, c_p$ using the above described Bernoulli trials (i.e., that $c'_k = c_k$ for all $k = 1, \ldots, p$)

Note that the above equivalence is a property of the cross-entropy and is not dependent on the "implementation" of $h[w_0, w_1](x_k)$ using the logistic sigmoid.

Support Vector Machines (SVM)

SVM Idea – Which Linear Classifier is the Best?



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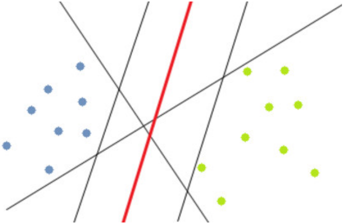

Benefits of maximum margin:

- Intuitively, the maximum margin is good w.r.t. generalization.
- Only the *support vectors* (those on the margin) matter; others can, in principle, be ignored.

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Notation:

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Consider a linear classifier:

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

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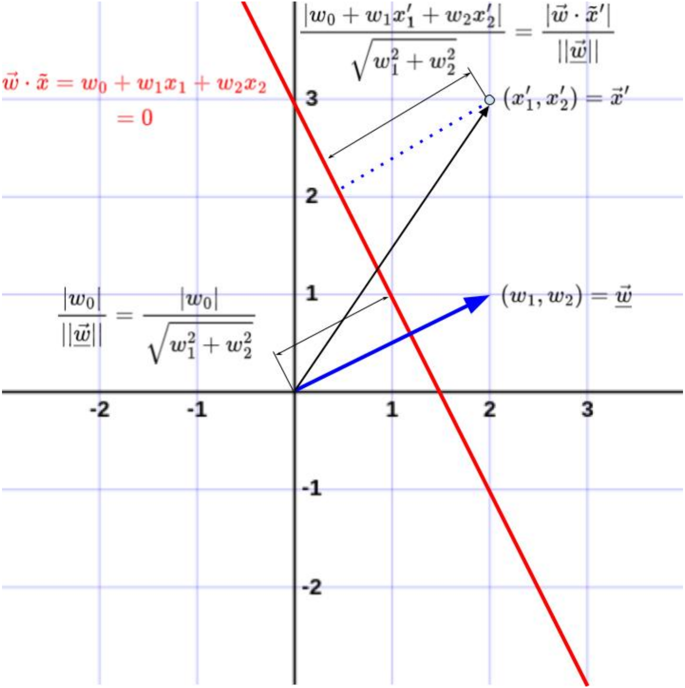
The *distance* of $\vec{x}$ from the separating hyperplane determined by $\vec{w}$ is

$$d[\vec{w}](\vec{x}) = \frac{|\vec{w} \cdot \tilde{\mathbf{x}}|}{\|\underline{\vec{w}}\|}$$

Recall that $\vec{w} \cdot \tilde{\mathbf{x}}$ is positive for $\vec{x}$ on the side to which $\underline{\vec{w}}$ points and negative on the opposite side.



$\frac{|w_0 + w_1 x'_1 + w_2 x'_2|}{\sqrt{w_1^2 + w_2^2}} = \frac{|\vec{w} \cdot \tilde{x}'|}{||\underline{\vec{w}}||}$
$\vec{w} \cdot \tilde{x} = w_0 + w_1 x_1 + w_2 x_2$
$= 0$
$(x'_1, x'_2) = \tilde{x}'$
$(w_1, w_2) = \underline{\vec{w}}$
$\frac{|w_0|}{||\underline{\vec{w}}||} = \frac{|w_0|}{\sqrt{w_1^2 + w_2^2}}$
3
2
1
-1
-2
-2
-1
1
2
3

Margin

- Given a training set

$$D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots, (\vec{x}_p, y_p)\}$$

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

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- Assume that D is linearly separable, let $\vec{w}$ *be consistent with* D.

  Margin of $\vec{w}$ is twice the minimum distance between feature vectors $\vec{x}_k$ and the separating hyperplane determined by $\vec{w}$, i.e.,

  $$2 \min_k d[\vec{w}](\vec{x}_k) = 2 \min_k \frac{|\vec{w} \cdot \tilde{\mathbf{x}}_k|}{\|\underline{\vec{w}}\|}$$

- Our goal is to find $\vec{w}$ consistent with D that maximizes the margin.

  Note that to maximize the margin it suffices to maximize $\min_k \frac{|\vec{w} \cdot \tilde{\mathbf{x}}_k|}{\|\underline{\vec{w}}\|}$ over $\vec{w}$ consistent with D.

Finding the Maximum Margin Classifier

We want to maximize the minimum distance of the feature vectors $\vec{x}_k$ from the separating hyperplane determined by $\vec{w}$.

Finding the Maximum Margin Classifier

We want to maximize the minimum distance of the feature vectors $\vec{x}_k$ from the separating hyperplane determined by $\vec{w}$.

Formally, we use the following:

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{|\vec{w} \cdot \tilde{\mathbf{x}}_k|}{||\underline{\vec{w}}||} \qquad \text{(= the distance of closest } \vec{x}_k\text{'s to the sep. hyperplane)}$$

over the following constraints

$\vec{w} \cdot \tilde{\mathbf{x}}_k > 0$ for all k satisfying $y_k = 1$

$\vec{w} \cdot \tilde{\mathbf{x}}_k < 0$ for all k satisfying $y_k = -1$

(the contraints make sure that $\vec{w}$ is consistent with the training set D)

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{|\vec{w} \cdot \tilde{\mathbf{x}}_k|}{||\underline{\vec{w}}||}$$

over the following constraints

$$\vec{w} \cdot \tilde{\mathbf{x}}_k > 0 \text{ for all } k \text{ satisfying } y_k = 1$$

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Can be made more succinct:

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k}{||\underline{\vec{w}}||} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) > 0$$

The reason is that $\vec{w}$ is consistent with D. That is, $\vec{w} \cdot \tilde{x}_k > 0$ for $y_k = 1$, and $\vec{w} \cdot \tilde{x}_k < 0$ for $y_k = -1$.

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) > 0$$

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Observation: For every $\vec{w}$ satisfying $\min_k(y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) > 0$ there is $\vec{w}'$ satisfying $\min_k(y_k \cdot \vec{w}' \cdot \tilde{\mathbf{x}}_k) = 1$ such that

$$\min_k \frac{y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k}{\|\underline{\vec{w}}\|} = \min_k \frac{y_k \cdot \vec{w}' \cdot \tilde{\mathbf{x}}_k}{\|\underline{\vec{w}}'\|}$$

Proof: Just consider $\vec{w}' = \vec{w}/\xi$ where $\xi = \min_k(y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k)$. □

To maximize the margin, find $\vec{w}$ *maximizing*

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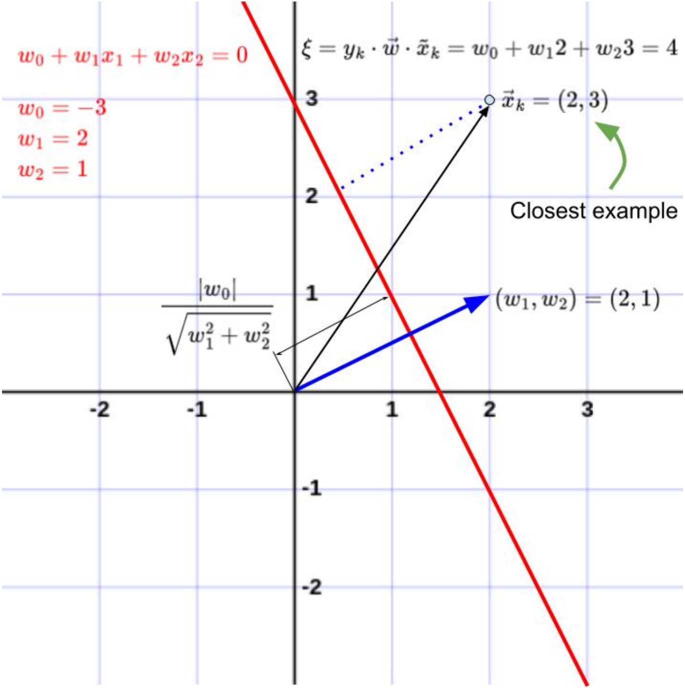
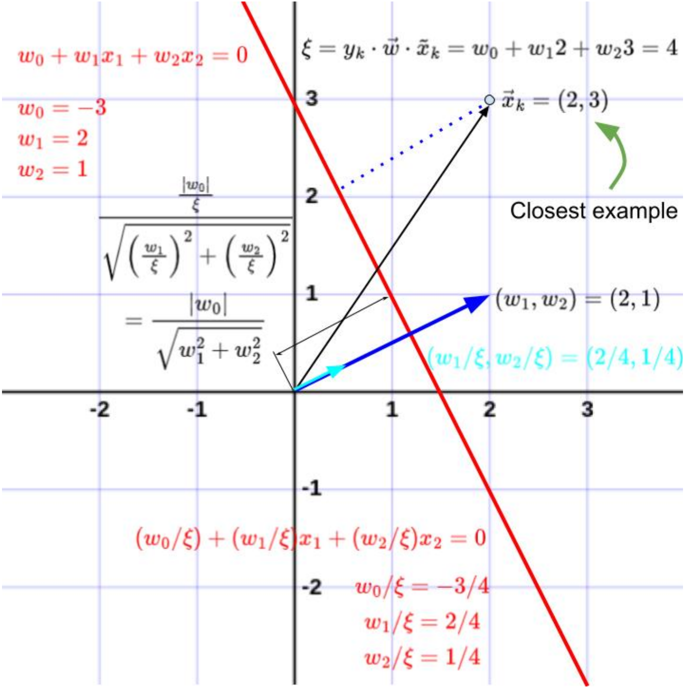


$w_0 + w_1x_1 + w_2x_2 = 0$
$w_0 = -3$
$w_1 = 2$
$w_2 = 1$
$\xi = y_k \cdot \vec{w} \cdot \tilde{x}_k = w_0 + w_1 2 + w_2 3 = 4$
$\vec{x}_k = (2, 3)$
Closest example
$(w_1, w_2) = (2, 1)$
$\frac{|w_0|}{\sqrt{w_1^2 + w_2^2}}$
3
2
1
-1
-2
-2
-1
1
2
3



$w_0 + w_1 x_1 + w_2 x_2 = 0$
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Closest example
$\frac{\frac{|w_0|}{\xi}}{\sqrt{\left(\frac{w_1}{\xi}\right)^2 + \left(\frac{w_2}{\xi}\right)^2}} = \frac{|w_0|}{\sqrt{w_1^2 + w_2^2}}$
$(w_1, w_2) = (2, 1)$
$(w_1/\xi, w_2/\xi) = (2/4, 1/4)$
$(w_0/\xi) + (w_1/\xi)x_1 + (w_2/\xi)x_2 = 0$
$w_0/\xi = -3/4$
$w_1/\xi = 2/4$
$w_2/\xi = 1/4$

To maximize the margin, find $\vec{w}$ *maximizing*

$$\min_k \frac{y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) = 1$$

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can be further simplified to

To maximize the margin, find $\vec{w}$ *maximizing*

$$\frac{1}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) = 1$$

To maximize the margin, find $\vec{w}$ *maximizing*

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$$\frac{1}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) = 1$$

Can be adjusted by loosening the constraints:

To maximize the margin, find $\vec{w}$ *maximizing*

$$\frac{1}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k (y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) \geq 1$$

If the latter is solved by $\vec{w}'$ with $\min_k(y_k \cdot \vec{w}' \cdot \tilde{\mathbf{x}}_k) > 1$, then

$$\min_k \frac{y_k \cdot \vec{w}' \cdot \tilde{\mathbf{x}}_k}{\left|\left|\underline{\vec{w}'}\right|\right|} > \frac{1}{\left|\left|\underline{\vec{w}'}\right|\right|} \geq \frac{1}{||\underline{\vec{w}}||} = \frac{\min_k y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k}{||\underline{\vec{w}}||}$$

For all $\vec{w}$ satisfying $\min_k(y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k) = 1$, which contradicts the fact that the maximum margin is attained by such a $\vec{w}$.

To maximize the margin, find $\vec{w}$ *maximizing*

$$\frac{1}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1$$

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$$\frac{1}{\|\underline{\vec{w}}\|} \quad \text{over} \quad \min_k y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1$$

Can be turned into

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$$||\underline{\vec{w}}|| \quad \text{over} \quad \min_k y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1$$

And, finally,

To maximize the margin, find $\vec{w}$ *minimizing*

$$\underline{\vec{w}} \cdot \underline{\vec{w}} \quad \text{over} \quad y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1 \text{ for all } k$$

Indeed, just note that $||\underline{\vec{w}}|| = \sqrt{\underline{\vec{w}} \cdot \underline{\vec{w}}}$.

SVM – Optimization

Assume a given training set

$$D = \{(\vec{x}_1, y_1)), (\vec{x}_2, y_2), \ldots, (\vec{x}_p, y_p)\}$$

Here $\vec{x}_k = (x_{k1} \ldots, x_{kn}) \in X \subseteq \mathbb{R}^n$ and $y_k \in \{-1, 1\}$.
(recall $\tilde{x}_k = (x_{k0}, x_{k1}, \ldots, x_{kn})$ where $x_{k0} = 1$)

Margin maximization as a *quadratic optimization problem:*

> Find $\vec{w}$ *minimizing*
>
> $$\underline{\vec{w}} \cdot \underline{\vec{w}}$$
>
> under the constraints
>
> $$y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1 \text{ for all } k$$

Support vectors are vectors $\vec{x}_k$ closest to the *optimal* separating hyperplane, i.e., those satisfying $y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k = 1$ for a minimizing $\vec{w}$.

Example

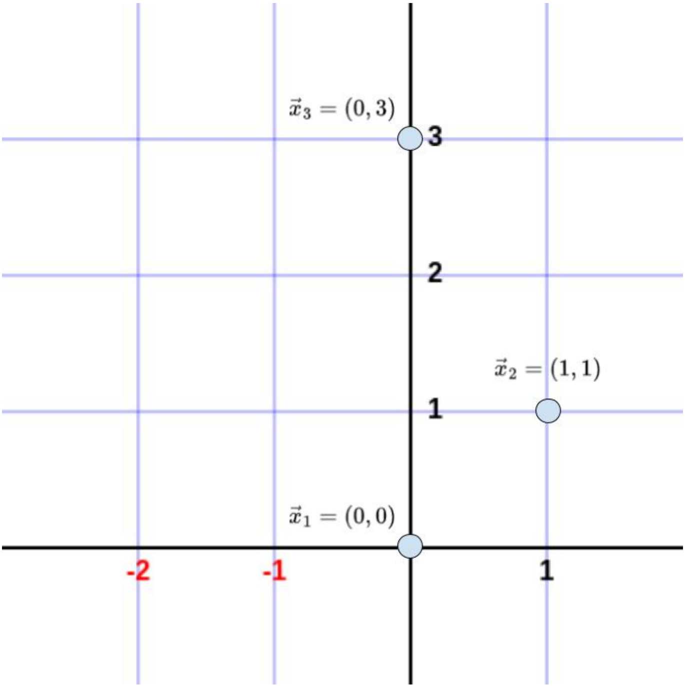
Training set:

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

That is

$$\begin{aligned} \vec{x}_1 &= (0,0) & \tilde{\mathbf{x}}_1 &= (1,0,0) \\ \vec{x}_2 &= (1,1) & \tilde{\mathbf{x}}_2 &= (1,1,1) \\ \vec{x}_3 &= (0,3) & \tilde{\mathbf{x}}_3 &= (1,0,3) \end{aligned}$$

$$\begin{aligned} y_1 &= -1 \\ y_2 &= 1 \\ y_3 &= 1 \end{aligned}$$


$\vec{x}_3 = (0,3)$
3
2
$\vec{x}_2 = (1,1)$
1
$\vec{x}_1 = (0,0)$
-2
-1
1

Find $\vec{w}$ minimizing $w_1^2 + w_2^2$ under the constraints

$$(-1) \cdot (1w_0 + 0w_1 + 0w_2) = -w_0 \geq 1$$
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It can be solved using a quadratic programming solver.

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To solve by hand, assume that we know that $\vec{x}_1$ and $\vec{x}_2$ are support vectors.

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$$-w_0 = 1$$
$$w_0 + w_1 + w_2 = 1$$
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Note that the equality constraints correspond to our assumption that $\vec{x}_1$ and $\vec{x}_2$ are support vectors.

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Substituting $w_2 = 2 - w_1$ into the quadratic function we obtain

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This reduces our problem to

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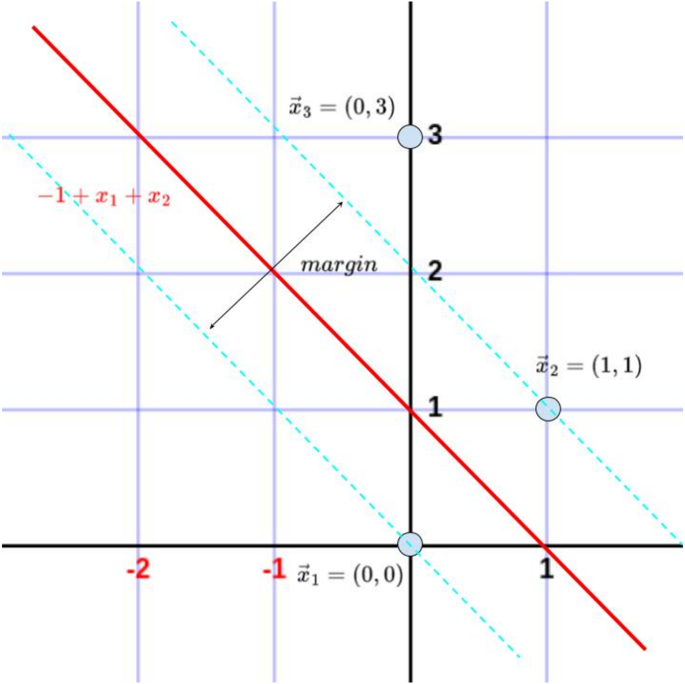
The final model is

$$h[\vec{w}](\vec{x}) = -1 + x_1 + x_2$$

The separating hyperplane is determined by

$$-1 + x_1 + x_2 = 0$$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The answer lies in their ability to deal with non-linearly separable sets efficiently using the *kernel trick* (see a later lecture).

Comments on Algorithms

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  - This iterative procedure decreases the (general) cost function.

Soft-margin SVM

Trade-off few misclassifications with a wide margin for the rest.

Find $\vec{w}$ *minimizing*

$$\underline{\vec{w}} \cdot \underline{\vec{w}} + C \sum_k \zeta_k$$

C is a hyperparameter

under the constraints

$$y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k \geq 1 - \zeta_k \text{ for all } k$$

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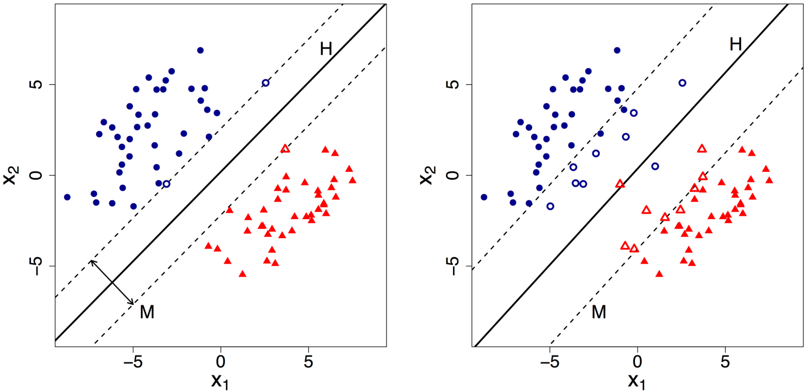
Which is the same as the following *unconstrained* optimization:

Find $\vec{w}$ *minimizing* the *hinge loss*

$$\underline{\vec{w}} \cdot \underline{\vec{w}} + C \sum_k \max(0, 1 - y_k \cdot \vec{w} \cdot \tilde{\mathbf{x}}_k)$$

Hard vs Soft Margin SVM



Source: Dishaa Agarwal

https://www.analyticsvidhya.com/blog/2021/04/insight-into-svm-support-vector-machine-along-with-code/

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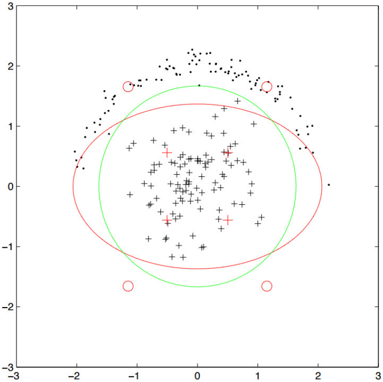
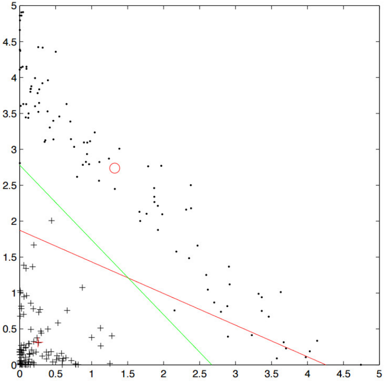
- SVMs can be applied to complex data types beyond feature vectors (e.g., graphs, sequences, relational data) by designing kernel functions for such data.
- SVM techniques have been extended to several tasks, such as regression [Vapnik et al. '97], principal component analysis [Schölkopf et al. '99], etc.

Kernel Methods

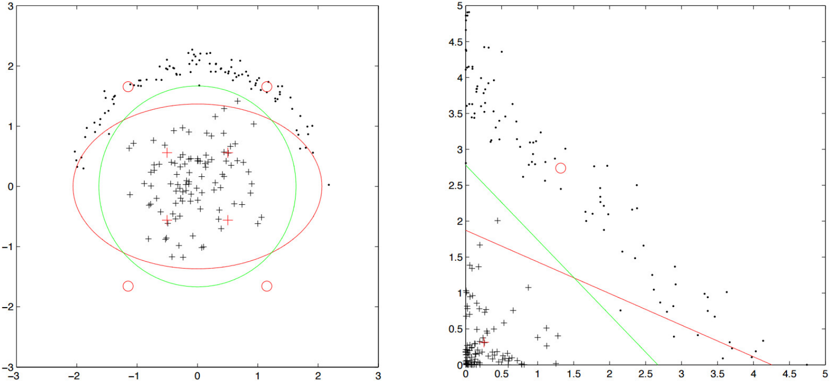
Quadratic Decision Boundary





Left: The original set,

Quadratic Decision Boundary



Left: The original set, Right: Transformed using the square of features.

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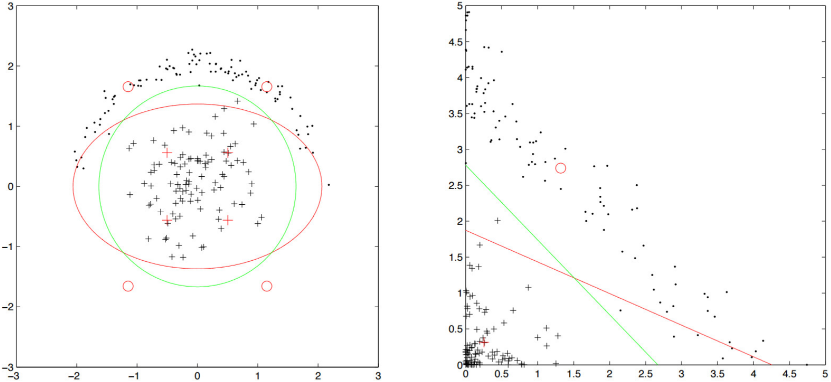

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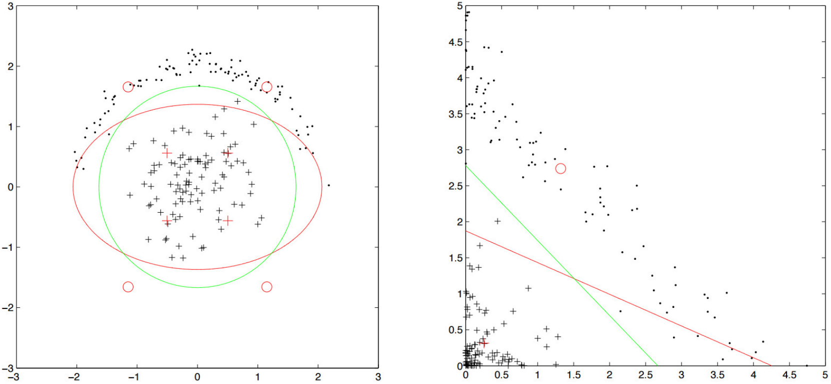

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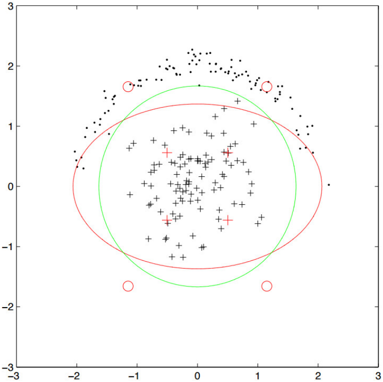

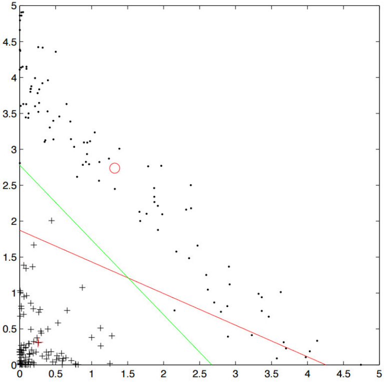

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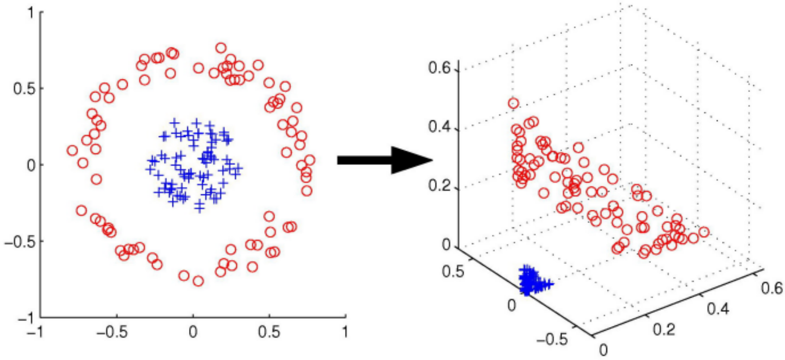
Another Solution



Mapping from $\mathbb{R}^2$ to $\mathbb{R}^3$ so that there is "more space" for linear separation.

Do We Need to Map Explicitly?

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To avoid explicit construction of the higher dimensional feature space, we use the so-called *kernel trick*.

But first, we need to *dualize* our learning algorithm.

Linear Regression

- Given a set D of training examples:

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

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

- **Our goal:** Find $\vec{w}$ so that $h[\vec{w}](\vec{x}_k) = \vec{w} \cdot \tilde{\mathbf{x}}_k$ is close to f_k for every $k = 1, \ldots, p$.

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

- **Squared Error Function:**

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

Regularized Linear Regression

Regularized Squared Error Function:

$$E(\vec{w}) \;=\; \frac{1}{2}\sum_{k=1}^{p}(\vec{w}\cdot\tilde{\mathbf{x}}_k - f_k)^2 + \vec{w}\cdot\vec{w}$$

Intuition: the added term $\vec{w}\cdot\vec{w}$ prevents growth of weights.

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The Representer Theorem: The weight vector $\vec{w}^*$ minimizing the regularized squared error function can be written as

$$\vec{w}^* = \sum_{i=1}^{p}\alpha_i f_i\,\tilde{\mathbf{x}}_i$$

Here $\alpha_1,\ldots,\alpha_p$ are suitable coefficients.

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Substituting this expression for weights in E gives

$$E'(\vec{w}^*) = \frac{1}{2}\sum_{k=1}^{p}\left(\sum_{i=1}^{p}\alpha_i f_i\,\tilde{\mathbf{x}}_i\cdot\tilde{\mathbf{x}}_k - f_k\right)^2 + \sum_{i=1}^{p}\sum_{j=1}^{p}\alpha_i\alpha_j f_i f_j\,\tilde{\mathbf{x}}_i\cdot\tilde{\mathbf{x}}_j$$

and we minimize E' w.r.t. $\alpha_1,\ldots,\alpha_p$. What is this good for??

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Find $\alpha_1, \ldots, \alpha_p$ *minimizing dual regularized squared error*

$$E'(\vec{w}^*) = \frac{1}{2} \sum_{k=1}^{p} \left(\sum_{i=1}^{p} \alpha_i f_i \, \tilde{\mathbf{x}}_i \cdot \tilde{\mathbf{x}}_k - f_k \right)^2 + \sum_{i=1}^{p} \sum_{j=1}^{p} \alpha_i \alpha_j f_i f_j \, \tilde{\mathbf{x}}_i \cdot \tilde{\mathbf{x}}_j$$

The resulting coefficients $\alpha_1, \ldots, \alpha_p$ give a weight vector

$$\vec{w}^* = \sum_{i=1}^{p} \alpha_i f_i \, \tilde{\mathbf{x}}_i$$

which in turn gives a linear model

$$h[\vec{w}^*](\vec{x}) = \vec{w}^* \tilde{\mathbf{x}} = \sum_{i=1}^{p} \alpha_i f_i \, \tilde{\mathbf{x}}_i \cdot \tilde{\mathbf{x}}$$

Note that all $\tilde{\mathbf{x}}, \tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_j, \tilde{\mathbf{x}}_k$ occur in dot products with themselves!

Find $\vec{\alpha} = (\alpha_1, \ldots, \alpha_p)$ *minimizing* *dual regularized squared error*

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Do we need to use the dot product in the above procedure? NO!

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Find $\vec{\alpha} = (\alpha_1, \ldots, \alpha_p)$ *minimizing* *kernel dual regularized squared error*

$$E'(\vec{w}^*) = \frac{1}{2}\sum_{k=1}^{p}\left(\sum_{i=1}^{p}\alpha_i f_i\, \kappa(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_k)) - f_k\right)^2 + \sum_{i=1}^{p}\sum_{j=1}^{p}\alpha_i\alpha_j f_i f_j\, \kappa(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_j)$$

Non-linear model: $h[\vec{\alpha}](\vec{x}) = \sum_{i=1}^{p}\alpha_i f_i\, \kappa(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}})$

Here κ is a **kernel function**. But now what is the trick?

Find $\vec{\alpha} = (\alpha_1, \ldots, \alpha_p)$ *minimizing dual regularized squared error*

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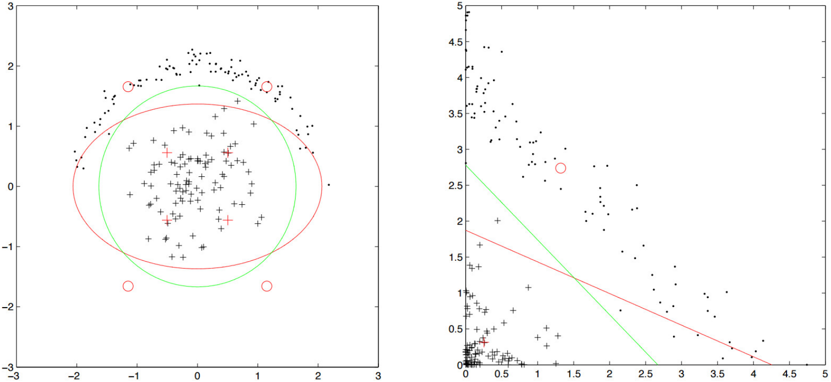
The trick is that suitable kernel functions κ correspond to dot products in transformed spaces!

Recall the Quadratic Decision Boundary



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THE Idea: Using the kernel $\kappa(\tilde{\mathbf{x}}_k, \tilde{\mathbf{x}}_\ell) = (\tilde{\mathbf{x}}_k \cdot \tilde{\mathbf{x}}_\ell)^2$ in the kernel, dual regularized squared error corresponds to using the regularized squared error after the transformation ϕ.

Quadratic Decision Boundary

Given a set D of training examples:

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

Assume that $f_i \in \{1, -1\}$ indicates the class of $\vec{x}_i$.

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Considering $\kappa(\tilde{\mathbf{x}}_k, \tilde{\mathbf{x}}_\ell) = (\tilde{\mathbf{x}}_k \cdot \tilde{\mathbf{x}}_\ell)^2$ in our kernel dual regularized squared error we obtain

Find $\vec{\alpha} = \alpha_1, \ldots, \alpha_p$ *minimizing*

$$E'(\vec{w}) = \frac{1}{2} \sum_{k=1}^{p} \left(\sum_{i=1}^{p} \alpha_i f_i \, (\tilde{\mathbf{x}}_i \cdot \tilde{\mathbf{x}}_k)^2 - f_k \right)^2 + \sum_{i=1}^{p} \sum_{j=1}^{p} \alpha_i \alpha_j f_i f_j \, (\tilde{\mathbf{x}}_i \cdot \tilde{\mathbf{x}}_j)^2$$

Non-linear classifier: $h[\vec{\alpha}](\vec{x}) = \sum_{i=1}^{p} \alpha_i f_i \, (\tilde{\mathbf{x}}_i \cdot \tilde{\mathbf{x}})^2$

Intuitively, minimizing E' in $\mathbb{R}^2$ gives a separating hyperplane for the input vectors transformed into $\mathbb{R}^5$. This means, that in $\mathbb{R}^2$ it searches for a quadratic (i.e., non-linear) boundary.

Examples of Kernels

- Linear: $\kappa(\tilde{\mathbf{x}}_\ell, \tilde{\mathbf{x}}_\mathbf{k}) = \tilde{\mathbf{x}}_\ell \cdot \tilde{\mathbf{x}}_\mathbf{k}$

  The corresponding mapping $\phi(\tilde{\mathbf{x}}) = \tilde{\mathbf{x}}$ is identity (no transformation).

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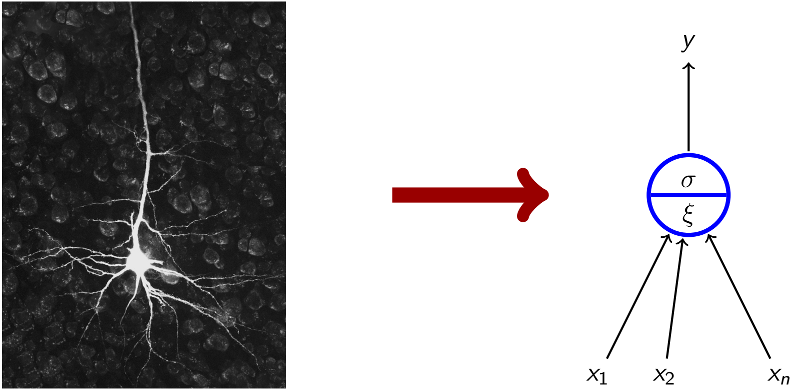
Choosing kernels remains to be the black magic of kernel methods. They are usually chosen based on trial and error (of course, experience and additional insight into data help).

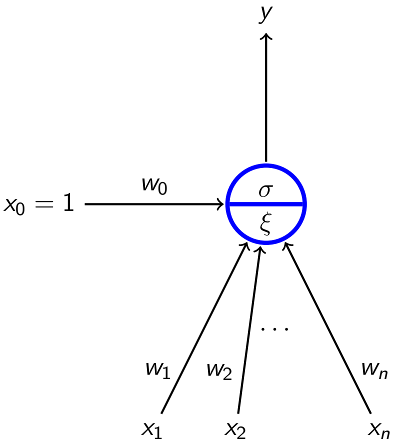
A similar trick can be done with (soft-margin) support vector machines.

Neural Networks

(Primitive) Mathematical Model of Neuron



Formal neuron



- $x_1, \ldots, x_n$ real *inputs*

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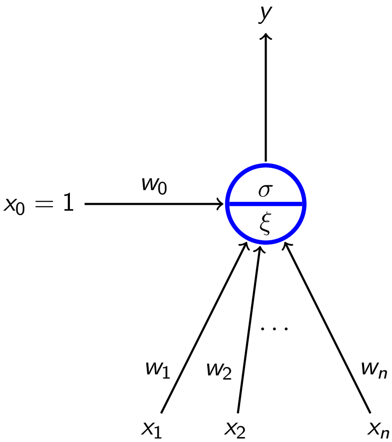
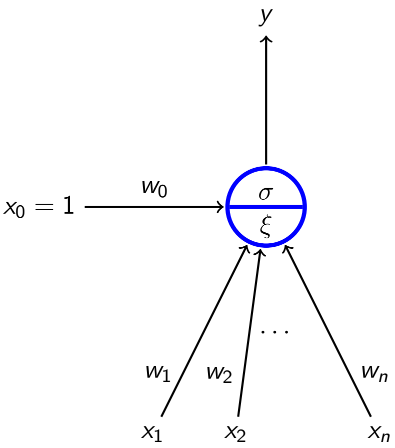


- $x_1, \dots, x_n$ real *inputs*
- x_0 special input, always 1

Formal neuron



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- $w_0, w_1, \dots, w_n$ real *weights*

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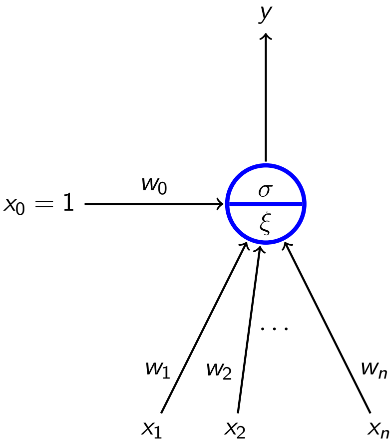

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  In general, other potentials are considered (e.g. Gaussian), more on this in PV021.

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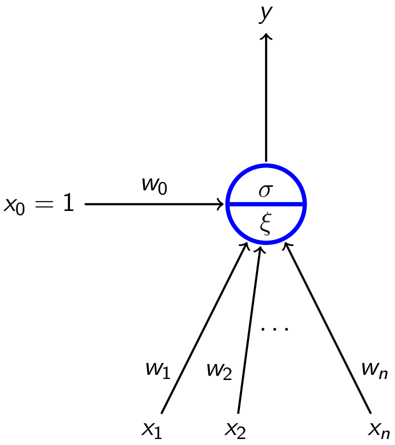

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  In general, other potentials are considered (e.g. Gaussian), more on this in PV021.
- y *output* defined by $y = \sigma(\xi)$ where σ is an *activation function*.

  We consider several activation functions.

  e.g., *linear threshold function*

$$\sigma(\xi) = sgn(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$$

Formal Neuron vs Linear Models

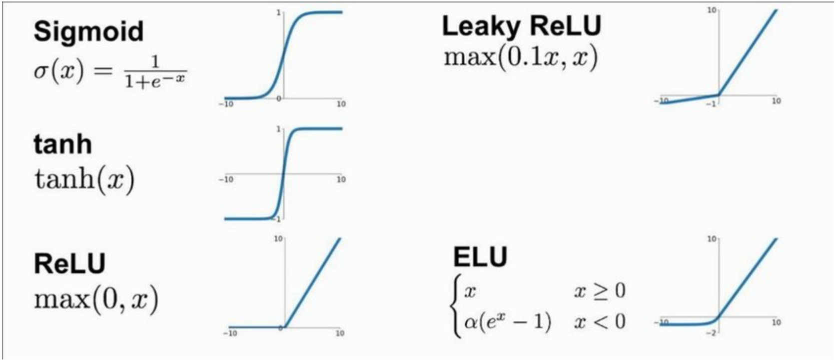
- If σ is a linear threshold function

  $$\sigma(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$$

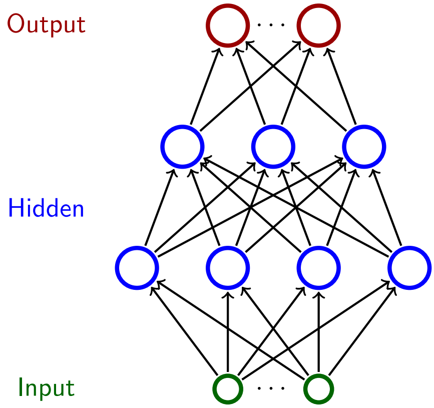
  We obtained a linear classifier.
- If σ is identity, i.e., $\sigma(\xi) = \xi$, we obtain a linear (affine) function.
- If $\sigma(\xi) = 1/(1 + e^{-\xi})$ we obtain the logistic regression.

Also, other activation functions are used in neural networks!

Activation Functions



Multilayer Perceptron (MLP)



- Neurons are organized in *layers* (input layer, output layer, possibly several hidden layers)
- Layers are numbered from 0; The input is 0-th
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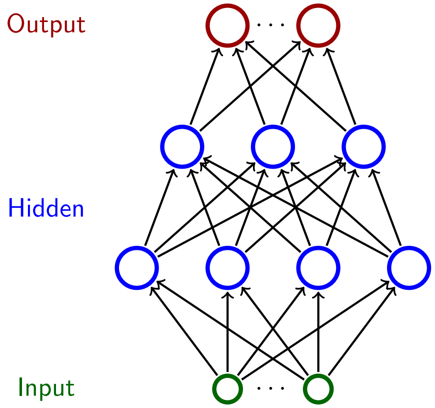

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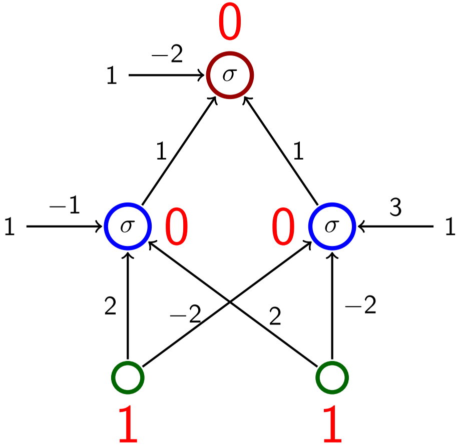
Intuition: The network computes a function: Assign input values to the input neurons and 0 to the rest. Proceed upwards through the layers, one layer per step. In the ℓ-th step consider output values of neurons in $\ell-1$-th layer as inputs to neurons of the ℓ-th layer. Compute output values of neurons in the ℓ-th layer.

Example



- Activation function: linear threshold

$$\sigma(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$$

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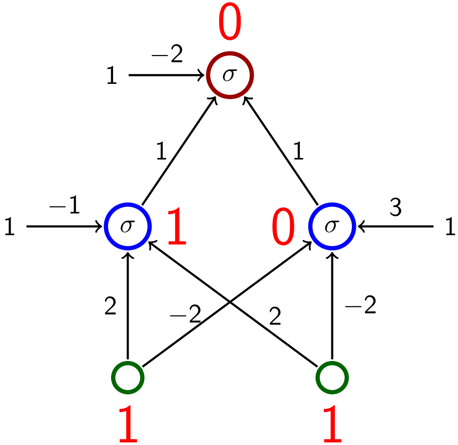

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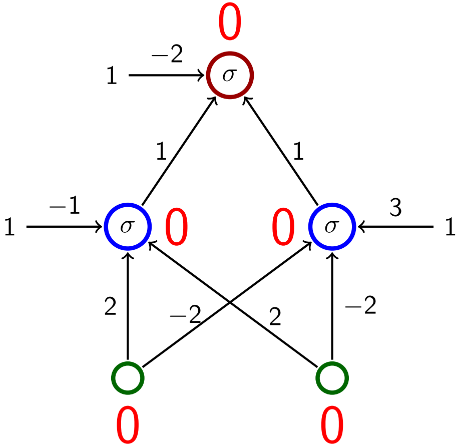

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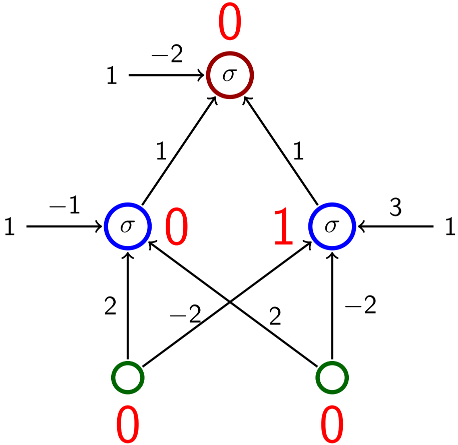

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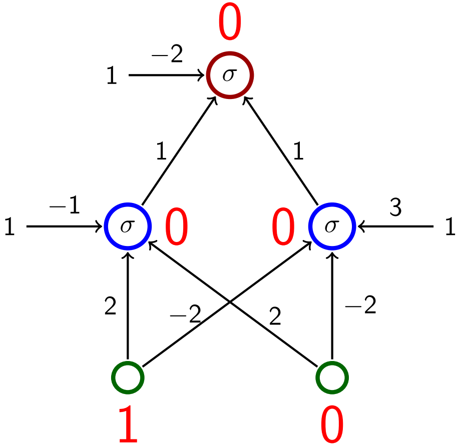

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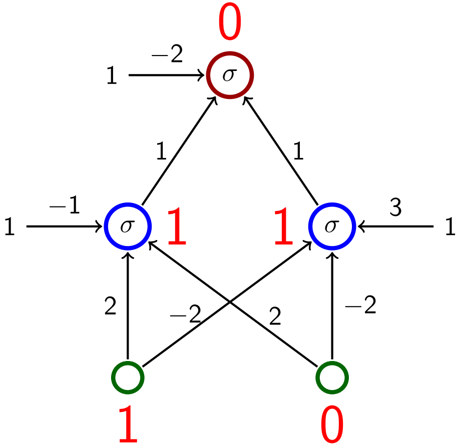

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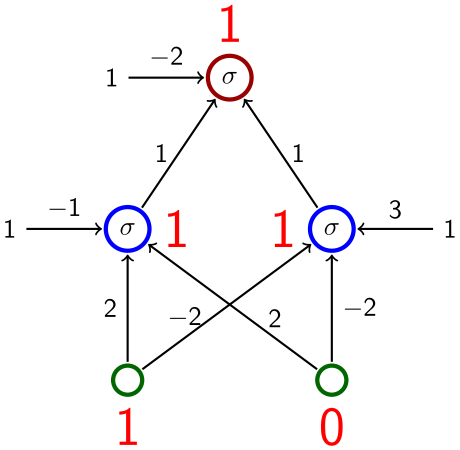

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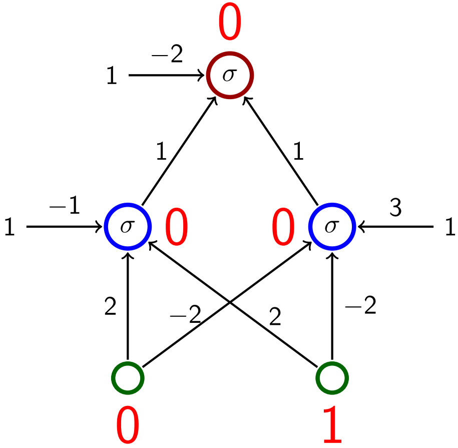

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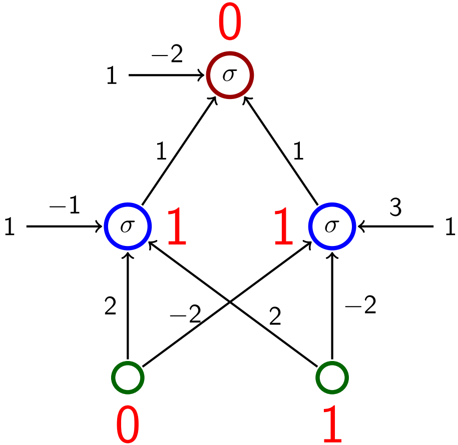

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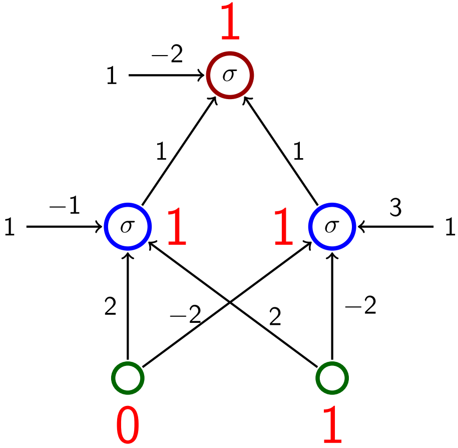

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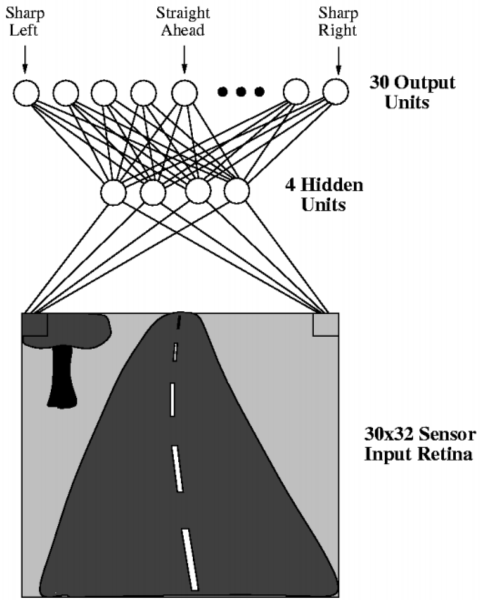
Classical Example – ALVINN

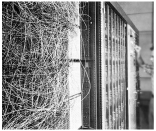


Source: `http://jmvidal.cse.sc.edu/talks/ann/alvin.html`

- One of the first autonomous car driving systems (in the 90s)
- ALVINN drives a car
- The net has $30 \times 32 = 960$ input neurons (the input space is $\mathbb{R}^{960}$).
- The value of each input captures the shade of gray of the corresponding pixel.
- Output neurons indicate where to turn (to the center of gravity).

A Bit of History

- Perceptron (Rosenblatt et al., 1957)



- Single layer (i.e., no hidden layers), the activation function *linear threshold*

  (i.e., a bit more general linear classifier)
- Perceptron learning algorithm
- Used to recognize digits

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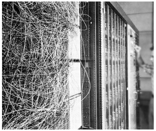

  - Single layer (i.e., no hidden layers), the activation function *linear threshold*

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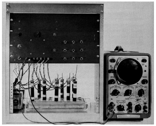
  - Perceptron learning algorithm
  - Used to recognize digits
- Adaline (Widrow & Hof, 1960)



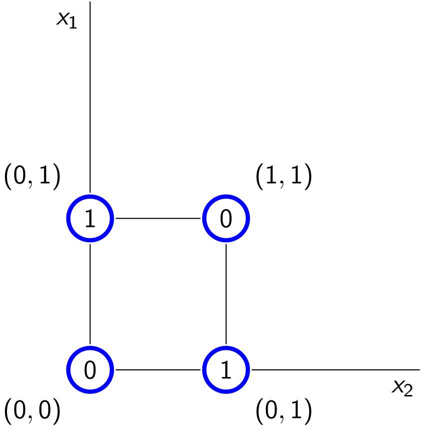
  - Single layer, the activation function *identity*

    (i.e., a bit more linear function)
  - Online version of the gradient descent
  - Used a new circuitry element called *memristor* which was able to "remember" history of current in form of resistance

In both cases, the expressive power is somewhat limited- it can only express linear decision boundaries and linear (affine) functions.

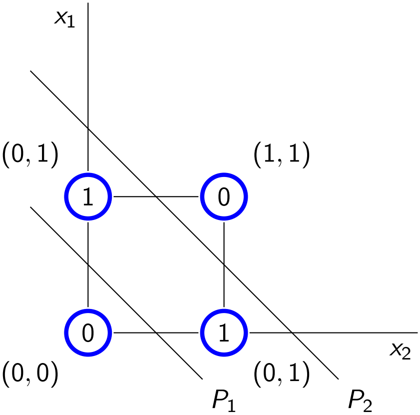
A Bit of History

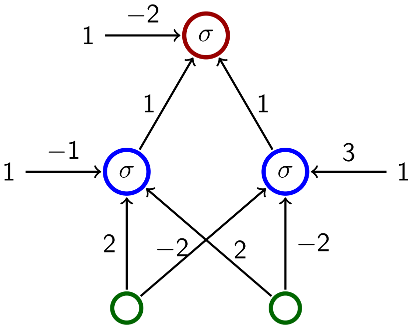
One of the famous (counter)-examples: XOR



No perceptron can distinguish between ones and zeros.

XOR vs Multilayer Perceptron





(Here, σ is a linear threshold function.)

$$P_1 : -1 + 2x_1 + 2x_2 = 0 \qquad P_2 : 3 - 2x_1 - 2x_2 = 0$$

The output neuron performs an intersection of half-spaces.

Boolean functions

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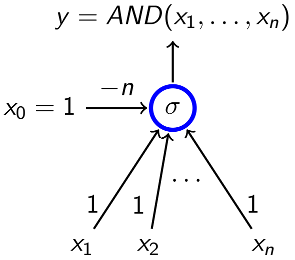
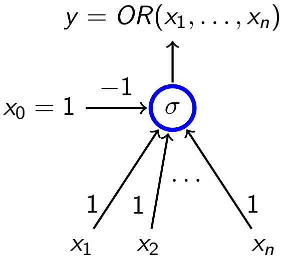
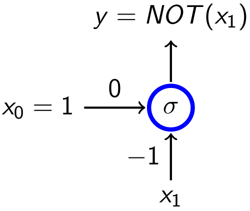
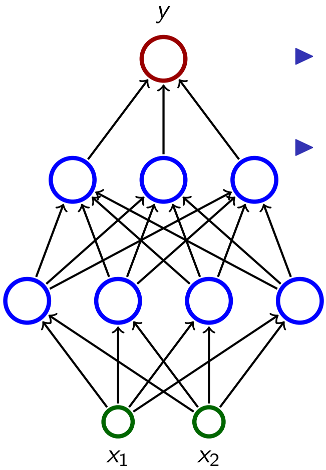






Non-linear separation



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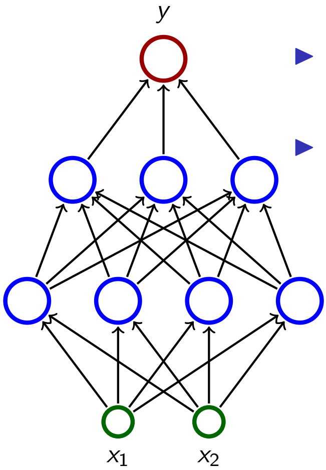

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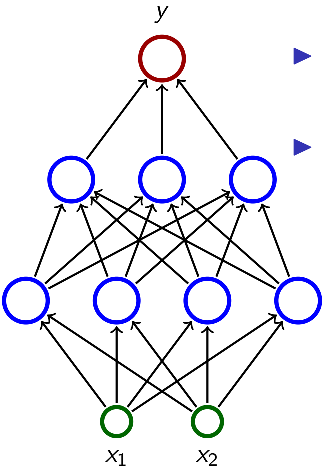

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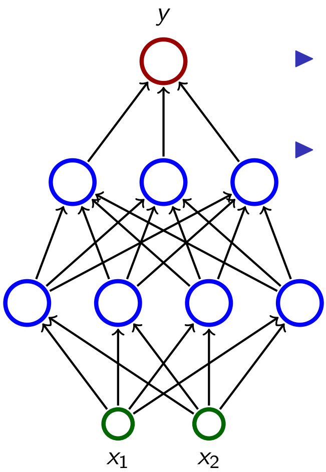

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  - The third layer may, e.g., make unions of some convex sets.

Example

Consider a triangle T in $\mathbb{R}^2$ determined by three vertices $(-1,-1),(1,-1),(-1,2)$.

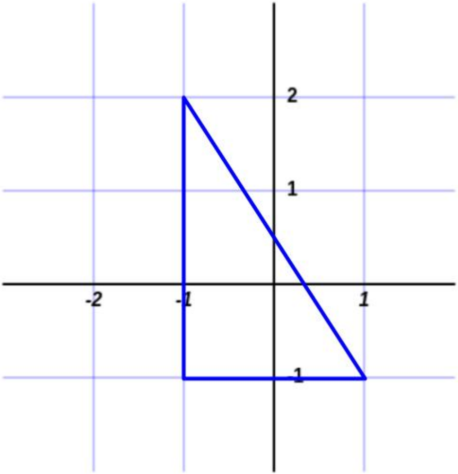
Give an example of a multilayer perceptron (MLP) with two input neurons and a single output neuron computing the function $F : \mathbb{R}^2 \to \{0,1\}$ defined as follows:

$F(x_1, x_2) = 1$ iff (x_1, x_2) lies either inside, or on the border of T

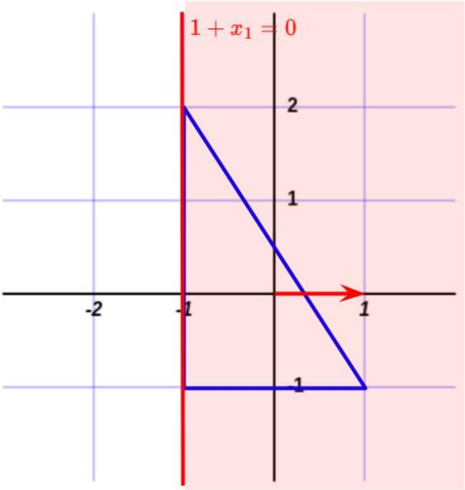
All activation functions in the network should be

$$\sigma(\xi) = sgn(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$$

Homework: Consider $F(x_1, x_2) = 1$ iff (x_1, x_2) lies inside of T (but *not* on the border)



2
1
-2
-1
1
-1


$1 + x_1 = 0$
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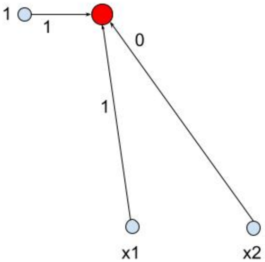
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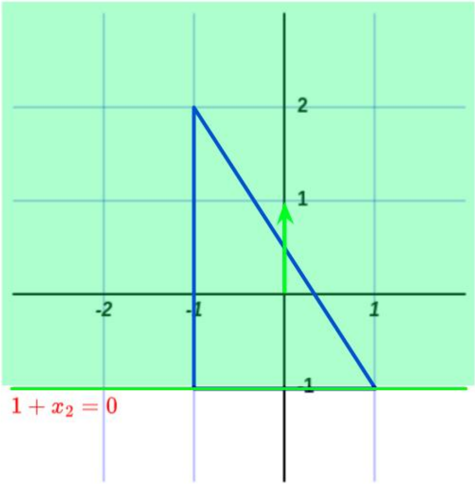
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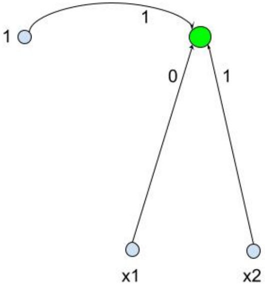
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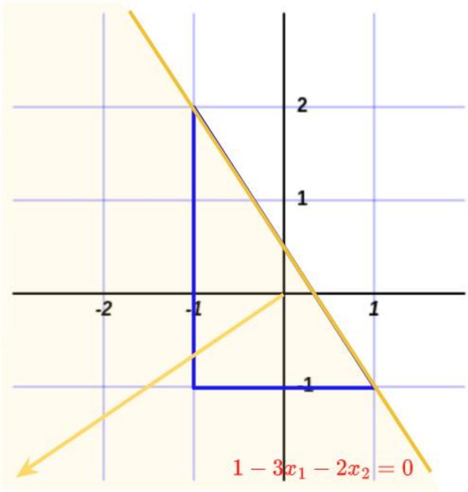
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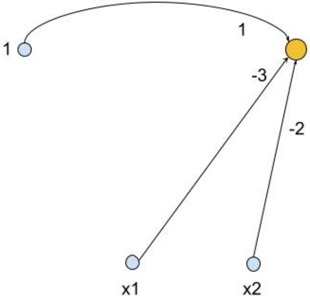
$1 - 3x_1 - 2x_2 = 0$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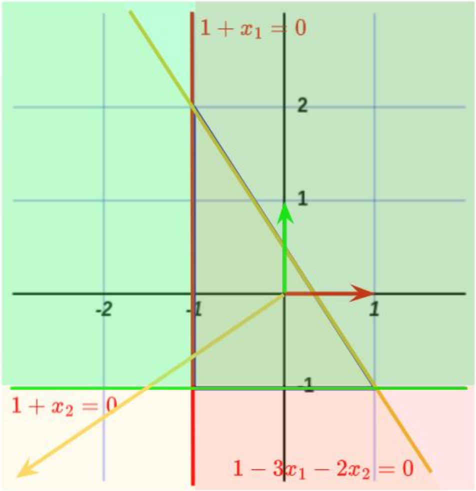

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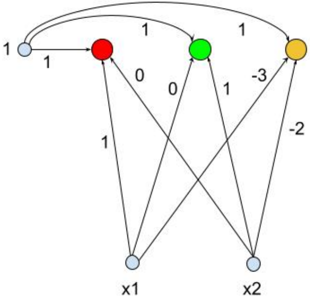

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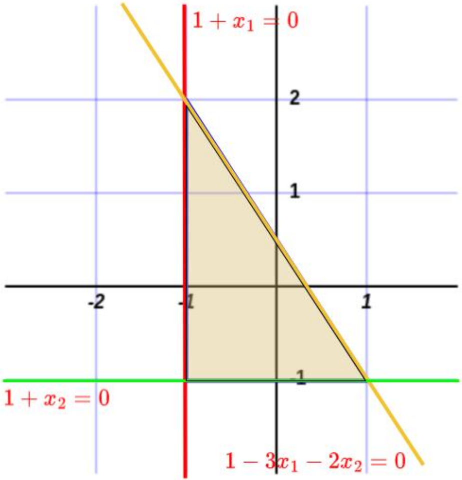

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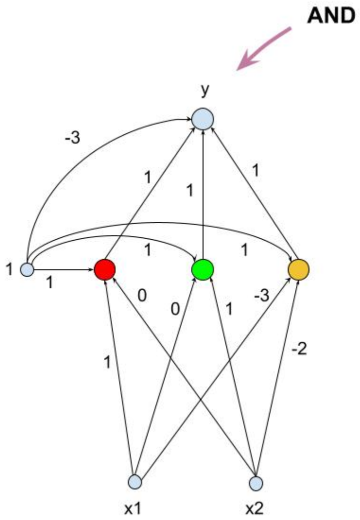

AND
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1
1
1
1
0
0
1
-3
-2
1
x1
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An efficient way of using the gradient descent was published in 1986!

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$$y_j = \sigma_j(\xi_j)$$

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- Fixing weights of all neurons, the network computes a function $F[\vec{w}] : \mathbb{R}^{|X|} \to \mathbb{R}^{|Y|}$ as follows: Assign values of a given vector $\vec{x} \in \mathbb{R}^{|X|}$ to the input neurons, evaluate the network, then $F[\vec{w}](\vec{x})$ is the vector of values of the output neurons.

  Here, we implicitly assume a fixed ordering on input and output vectors.

MLP – Learning

- Given a set D of training examples:

$$D = \left\{ \left(\vec{x}_k, \vec{d}_k\right) \quad \middle| \quad k = 1, \ldots, p \right\}$$

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- **Error Function:** $E(\vec{w})$ where $\vec{w}$ is a vector of all weights in the network. The choice of E depends on the solved task (classification vs regression etc.).

Example (Squared error):

$$E(\vec{w}) = \sum_{k=1}^{p} E_k(\vec{w})$$

where

$$E_k(\vec{w}) = \frac{1}{2} \sum_{j \in Y} (y_j[\vec{w}](\vec{x}_k) - d_{kj})^2$$

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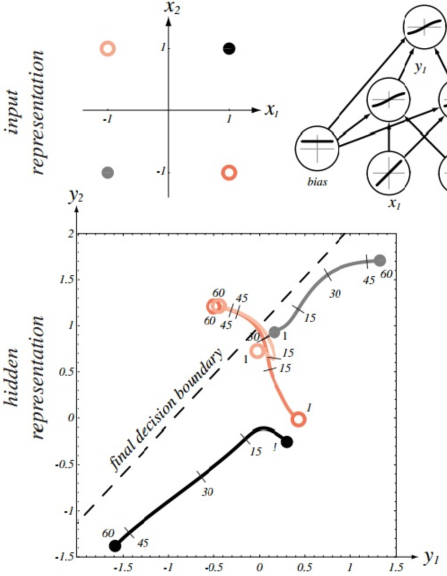
Note that $\frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t)})$ is a component of ∇E, i.e., the weight change in the step $t+1$ can be written as follows: $\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon(t) \cdot \nabla E(\vec{w}^{(t)})$.

Illustration of Gradient Descent – XOR



Source: Pattern Classification (2nd Edition); Richard O. Duda, Peter E. Hart, David G. Stork

Stochastic Gradient Descent (SGD)

Assume that $E(\vec{w}) = \sum_{k=1}^{p} E_k(\vec{w})$ where $E_k(\vec{w})$ is an error w.r.t. the single training example $(\vec{x}_k, \vec{d}_k)$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:
  - Choose (randomly) a set of training examples $T \subseteq \{1, \ldots, p\}$
  - Compute

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} + \Delta\vec{w}^{(t)}$$

where

$$\Delta\vec{w}^{(t)} = -\varepsilon(t) \cdot \sum_{k \in T} \nabla E_k(\vec{w}^{(t)})$$

- $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t+1$
- $\nabla E_k(\vec{w}^{(t)})$ is the gradient of the error of the example k

Note that the random choice of the minibatch is typically implemented by randomly shuffling all data and then choosing minibatches sequentially.

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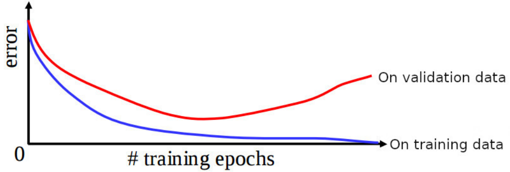
- In practice, does converge to low error for many large networks on (big) real data.
- Many epochs (thousands) may be required, hours or days of training for large networks.

There are many issues concerning learning efficiency (data normalization, selection of activation functions, weight initialization, learning rate, efficiency of the gradient descent itself, etc.) – see PV021.

Overfitting

- Due to their expressive power, neural networks are quite sensitive to overfitting.



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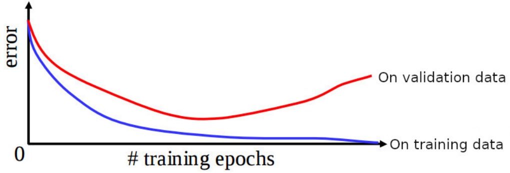

- Keep a hold-out validation set and test the error of the network on this set after every epoch. Stop training when additional epochs increase the validation error.

  The validation error can be measured by completely different means than the training error E.

Hidden Neurons Representations

Trained hidden neurons can be seen as newly constructed features.

E.g., in a two-layer network used for classification, the hidden layer transforms the input so that important features become explicit (and hence the result may become linearly separable).

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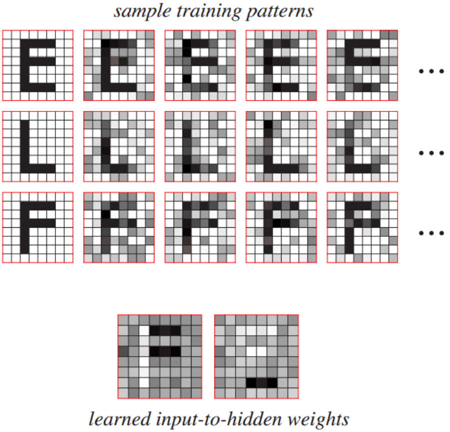
Consider a two-layer MLP, 64-2-3, for classifying letters (three output neurons, each corresponding to one of the letters).



Optimal Architecture?

- For MLP: Too few hidden neurons prevent the network from adequately fitting the data. Too many hidden units can result in overfitting.

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- There are (almost) infinitely many types of architectures of neural networks (convolutional, recurrent, transformers, adversarial, etc.) suitable for various tasks.
- **Transfer learning:** Start with a known solution to a related problem.

  Simplified view: Preserve lower parts of the network trained to solve the related problem (feature extractors). Add your top part and then train only the new top part (or train the whole network but carefully).

How to Choose Activation Functions & Error

- **Hidden neurons:** "Almost" linear activations such as (leaky) ReLU ($y = \max(0, \xi)$)

  Better than sigmoidal that saturate more often.
- **Output neurons:** Single output:
  - Regression: Typically "linear" output, i.e., no activation on the output neuron.
  - Binary classification: Logistic sigmoid $y = 1/(1 + e^{-\xi})$
- **Error:** Single output:
  - Regression: (Mean) squared error
  - Binary classification: Binary cross-entropy

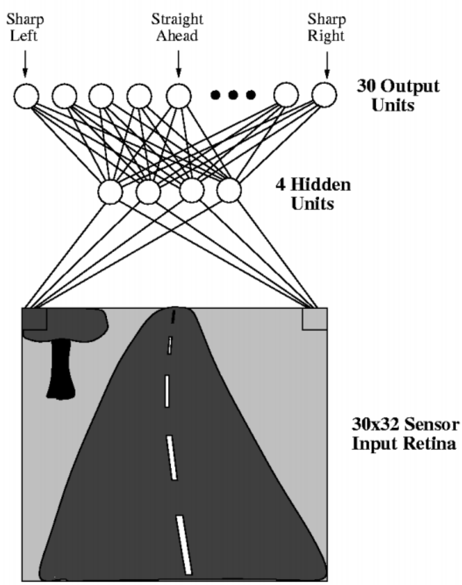
For multiple outputs and classification, use softmax output and cross-entropy.

Applications

- Image recognition, segmentation, etc.
- Machine translation and other text processing
- Text generation, image generation, movie generation, theatre plays generation
- Text to Speech and vice versa
- Finance, business predictions, fraud detection
- Game playing (backgammon is a classic example, AlphaGo is the famous one, computer games are the big ones, **bridge** is the hard one)
- (artificial brain and intelligence)
- ...

Text and image processing are possibly the most advanced deep learning applications.

ALVINN



Sharp Left
Straight Ahead
Sharp Right
30 Output Units
4 Hidden Units
30x32 Sensor Input Retina

ALVINN

- Two layer MLP, $960 - 4 - 30$ (sometimes $960 - 5 - 30$)

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- Sigmoidal activation function (logistic sigmoid).
- Direction corresponds to the center of gravity.

  , I.e., output neurons are considered as points of mass evenly distributed along a line. The weight of each neuron corresponds to its value.

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  - $\vec{d}_k \approx$ corresponding direction of the steering wheel set by the driver
- the values $\vec{d}_k$ computed using Gaussian distribution:

$$d_{ki} = e^{-D_i^2/10}$$

Where D_i is the distance between the i-th output from the one corresponding to the steering wheel's real direction.

(The authors claimed this approach is better than the binary output because similar road directions induce similar driver reactions.)

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Naive approach: just take images from the camera.

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- Images are very similar (the network sees the road from the right lane), overfitting.

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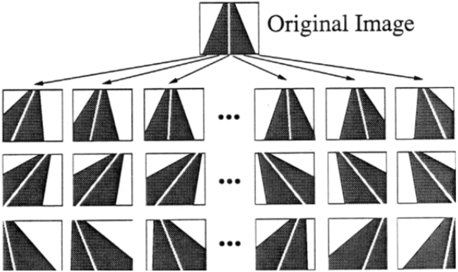

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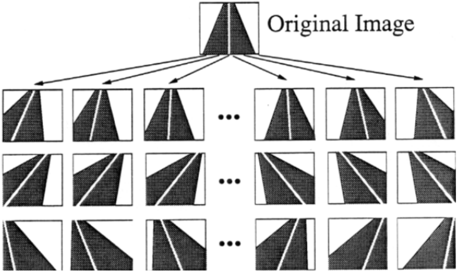

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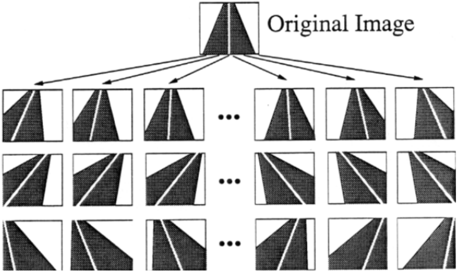

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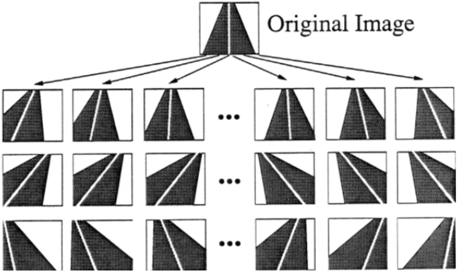

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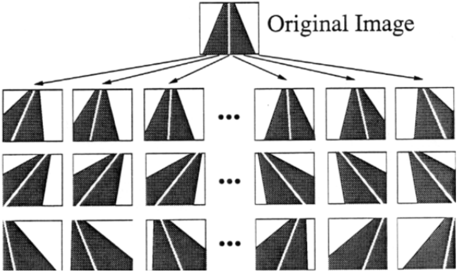

The repetitiveness of images was solved as follows:

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- afterward, a new image is captured, 15 copies made, and these new 15 substitute 15 selected from the buffer (10 with the smallest training error, five randomly)

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The result:

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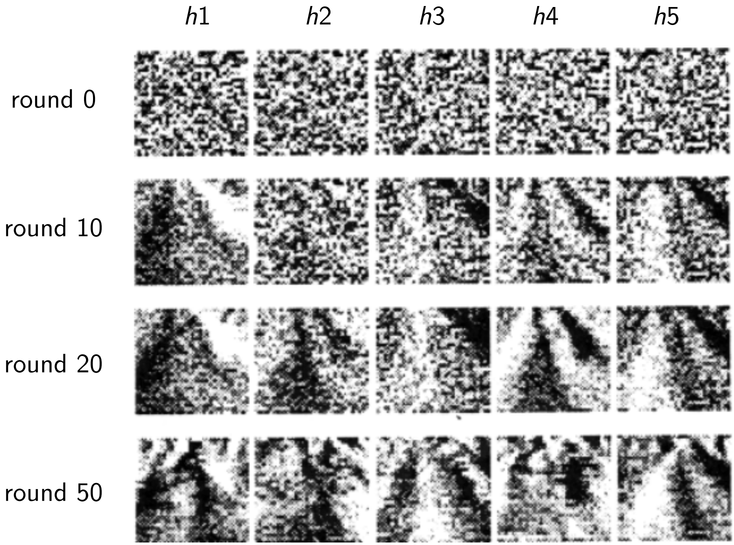
- ALVINN was able to go through roads it had never "seen" and in different weather

ALVINN – Weight Learning



Here $h1, \ldots, h5$ are values of hidden neurons.

Backpropagation

How to Compute the Gradient?

To implement a single step of the gradient descent, we need to compute the partial derivatives $\frac{\partial E}{\partial w_{ij}}$ of E w.r.t. all weights w_{ij}.

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  (i.e., not vectors as in the general case).
- The error function is the squared error.
  - Assume that 1 is the output neuron,
  - which means that $y_1 = y_1[\vec{w}](x)$ is the output of the network with weights $\vec{w}$ and the input x,
  - and the error on D is then

$$E(\vec{w}) = \frac{1}{2}(y_1 - d)^2$$

$$D = \{(x, d)\}$$

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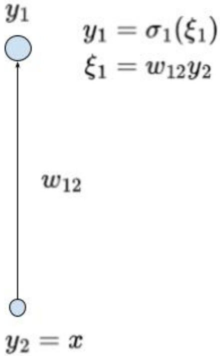

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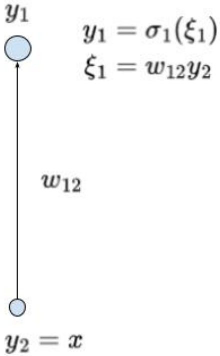

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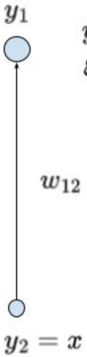

$$y_1 = \sigma_1(\xi_1)$$
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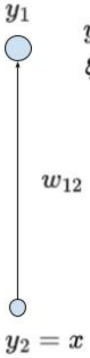

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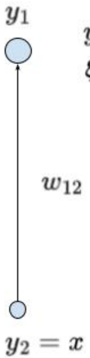

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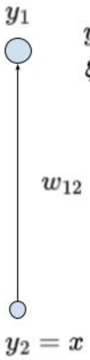

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Note that if σ_1 is identity, we obtain exactly the gradient from the linear regression method. Considering σ_1 equal to the logistic sigmoid and E the cross-entropy, we get the logistic regression gradient.

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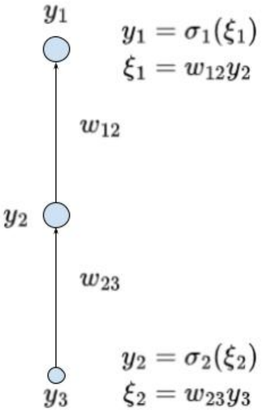

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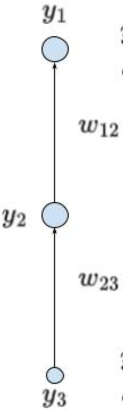

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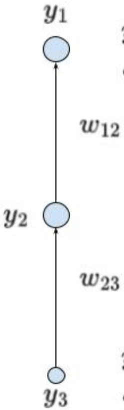

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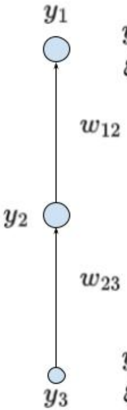

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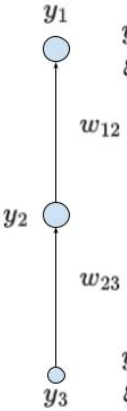

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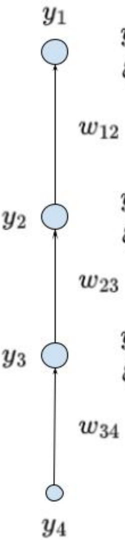

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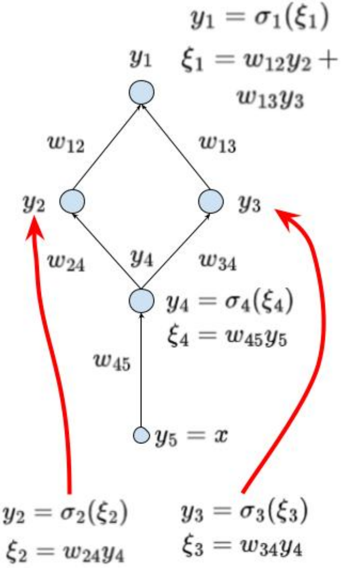

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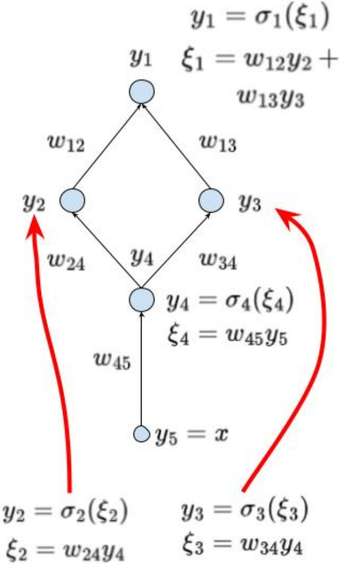

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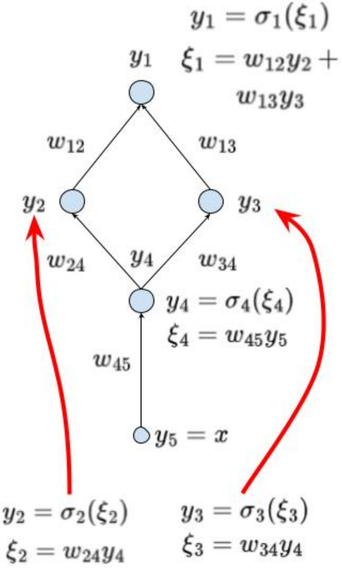

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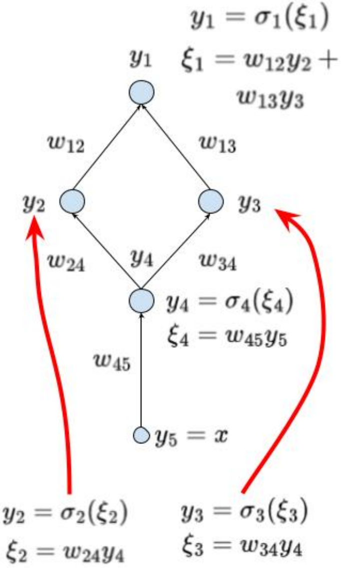

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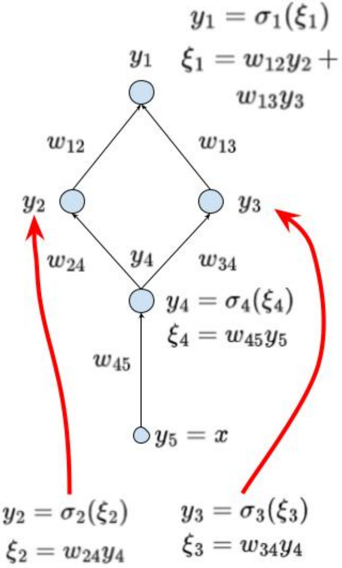

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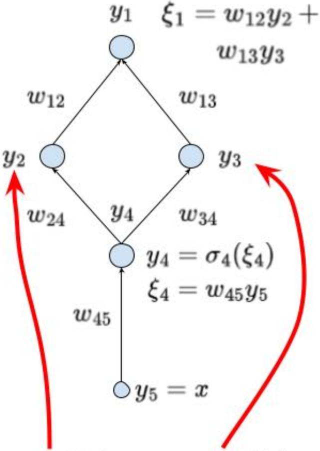
$$y_1 = \sigma_1(\xi_1)$$

$$\xi_1 = w_{12}y_2 + w_{13}y_3$$



$$y_4 = \sigma_4(\xi_4)$$

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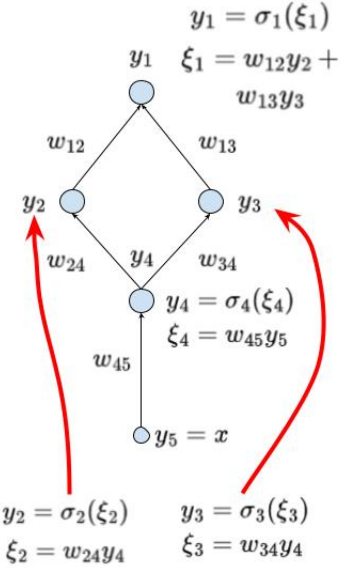
$$\frac{\partial E}{\partial w_{45}} = \frac{\partial E}{\partial y_4}\frac{\partial y_4}{\partial \xi_4}\frac{\partial \xi_3}{\partial w_{45}} = \frac{\partial E}{\partial y_4}\sigma_4'(\xi_4)y_5$$

$$D = \{(x, d)\}$$

$$E = \frac{1}{2}(y_1 - d)^2$$



$$\frac{\partial E}{\partial y_1} = y_1 - d$$

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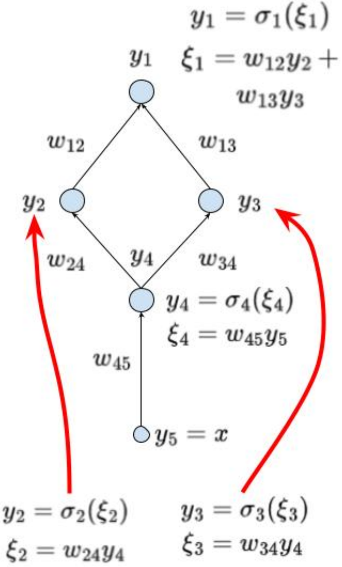

$$\frac{\partial E}{\partial y_1} = y_1 - d$$

$$\frac{\partial E}{\partial y_2} = \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial \xi_1}\frac{\partial \xi_1}{\partial y_2} = \frac{\partial E}{\partial y_1}\sigma_1'(\xi_1)w_{12}$$

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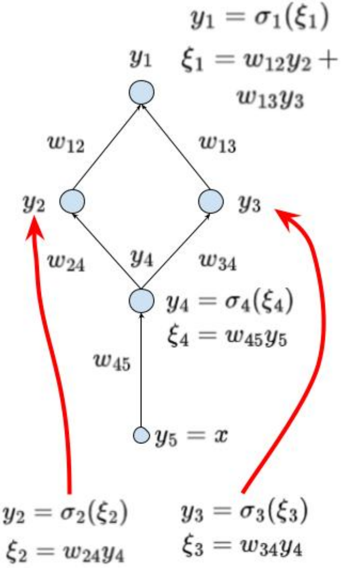

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$$\frac{\partial E}{\partial y_3} = \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial \xi_1}\frac{\partial \xi_1}{\partial y_3} = \frac{\partial E}{\partial y_1}\sigma_1'(\xi_1)w_{13}$$

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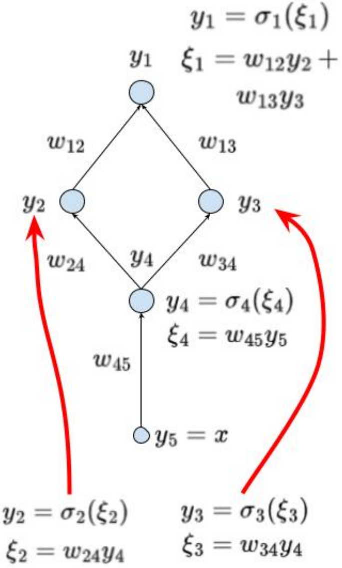

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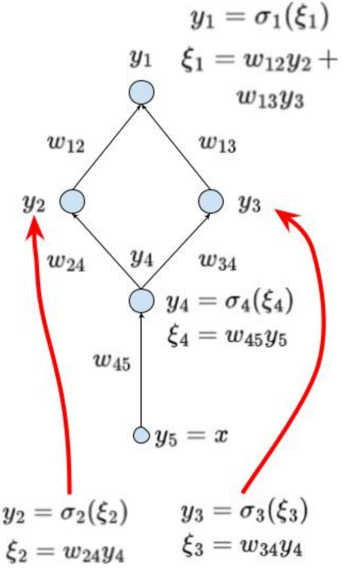

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$$\frac{\partial E}{\partial y_4}$$

$$D = \{(x, d)\}$$

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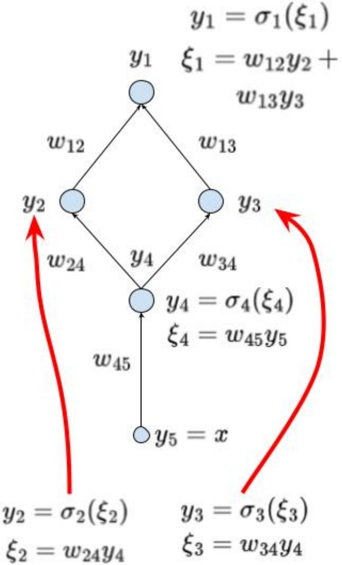

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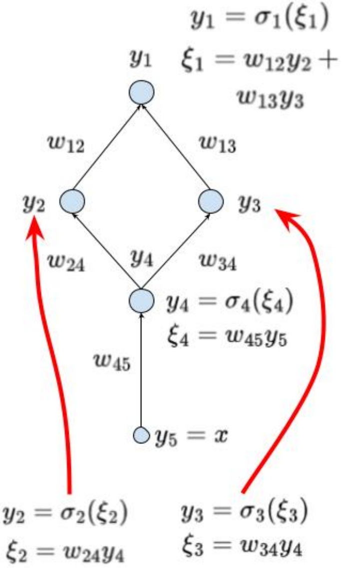
$$\frac{\partial E}{\partial y_4} = \frac{\partial E}{\partial y_2}\frac{\partial y_2}{\partial y_4} + \frac{\partial E}{\partial y_3}\frac{\partial y_3}{\partial y_4}$$

$$D = \{(x, d)\}$$

$$E = \frac{1}{2}(y_1 - d)^2$$



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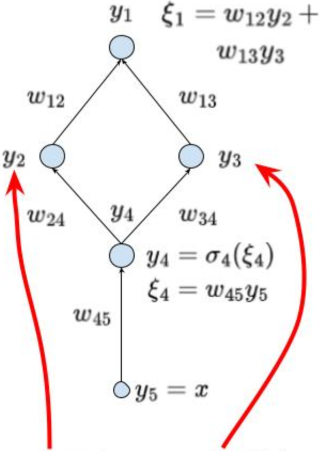
$$D = \{(x, d)\}$$

$$E = \frac{1}{2}(y_1 - d)^2$$

$$y_1 = \sigma_1(\xi_1)$$

$$\xi_1 = w_{12}y_2 + w_{13}y_3$$



$$y_4 = \sigma_4(\xi_4)$$

$$\xi_4 = w_{45}y_5$$

$$y_2 = \sigma_2(\xi_2) \qquad y_3 = \sigma_3(\xi_3)$$

$$\xi_2 = w_{24}y_4 \qquad \xi_3 = w_{34}y_4$$

$$\frac{\partial E}{\partial y_1} = y_1 - d$$

$$\frac{\partial E}{\partial y_2} = \frac{\partial E}{\partial y_1}\frac{\partial y_1}{\partial \xi_1}\frac{\partial \xi_1}{\partial y_2} = \frac{\partial E}{\partial y_1}\sigma_1'(\xi_1)w_{12}$$

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$$\begin{aligned}\frac{\partial E}{\partial y_4} &= \frac{\partial E}{\partial y_2}\frac{\partial y_2}{\partial y_4} + \frac{\partial E}{\partial y_3}\frac{\partial y_3}{\partial y_4} \\ &= \frac{\partial E}{\partial y_2}\frac{\partial y_2}{\partial \xi_2}\frac{\partial \xi_2}{\partial y_4} + \frac{\partial E}{\partial y_3}\frac{\partial y_3}{\partial \xi_3}\frac{\partial \xi_3}{\partial y_4} \\ &= \frac{\partial E}{\partial y_2}\sigma_2'(\xi_2)w_{24} + \frac{\partial E}{\partial y_3}\sigma_3'(\xi_3)w_{34}\end{aligned}$$

MLP – Gradient Computation

Under our simplifying assumptions $D = \{(x, d)\}$ and $E = (y_1 - d)^2$ the gradient computaton proceeds as follows:

Applying the chain rule, we obtain

$$\frac{\partial E_k}{\partial w_{ji}} = \frac{\partial E_k}{\partial y_j} \cdot \sigma_j'(\xi_j) \cdot y_i$$

where (after more applications of the chain rule)

$$\frac{\partial E_k}{\partial y_1} = y_1 - d$$

Keep in mind that 1 is the only output neuron which means that y_1 is the value of the network.

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot w_{rj} \qquad \text{for } j \in Z \smallsetminus (Y \cup X)$$

Here $y_r = y[\vec{w}](x)$ where $\vec{w}$ are the current weights and x is the example input.

MLP – Gradient Computation – General!

Let us drop our simplifying assumptions!

- Given a set D of training examples:

$$D = \left\{ \left(\vec{x}_k, \vec{d}_k\right) \quad \middle| \quad k = 1, \ldots, p \right\}$$

Here $\vec{x}_k \in \mathbb{R}^{|X|}$ and $\vec{d}_k \in \mathbb{R}^{|Y|}$. We write d_{kj} to denote the value in $\vec{d}_k$ corresponding to the output neuron j.

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- **Error Function:** $E(\vec{w})$ where $\vec{w}$ is a vector of all weights in the network. The choice of E depends on the solved task (classification vs regression, etc.).

Example (Squared error):

$$E(\vec{w}) = \sum_{k=1}^{p} E_k(\vec{w})$$

where

$$E_k(\vec{w}) = \frac{1}{2} \sum_{j \in Y} \left(y_j[\vec{w}](\vec{x}_k) - d_{kj}\right)^2$$

MLP – Gradient Computation

For every weight w_{ji} we have (obviously)

$$\frac{\partial E}{\partial w_{ji}} = \sum_{k=1}^{p} \frac{\partial E_k}{\partial w_{ji}}$$

So now it suffices to compute $\frac{\partial E_k}{\partial w_{ji}}$, that is the error for a fixed training example $(\vec{x}_k, \vec{d}_k)$.

MLP – Gradient Computation

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Applying the chain rule, we obtain

$$\frac{\partial E_k}{\partial w_{ji}} = \frac{\partial E_k}{\partial y_j} \cdot \sigma_j'(\xi_j) \cdot y_i$$

where (more applications of the chain rule)

$$\frac{\partial E_k}{\partial y_j} \text{ is computed directly for the output neurons } j \in Y$$

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot w_{rj} \qquad \text{for } j \in Z \setminus (Y \cup X)$$

(Here $y_r = y[\vec{w}](\vec{x}_k)$ where $\vec{w}$ are the current weights and $\vec{x}_k$ is the input of the k-th training example.)

MLP – Backpropagation

Input: A training set $D = \left\{ \left(\vec{x}_k, \vec{d}_k\right) \quad \middle| \quad k = 1, \ldots, p \right\}$ and the current vector of weights $\vec{w}$.

Note that the backprop. is repeated in every iteration of the gradient descent!

- Evaluate all values y_i of neurons using the standard bottom-up procedure with the input $\vec{x}_k$.

MLP – Backpropagation

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Note that the backprop. is repeated in every iteration of the gradient descent!

- Evaluate all values y_i of neurons using the standard bottom-up procedure with the input $\vec{x}_k$.
- For every training example $(\vec{x}_k, \vec{d}_k)$ compute $\frac{\partial E_k}{\partial y_j}$ using *backpropagation* through layers top-down :
  - For all $j \in Y$ compute $\frac{\partial E_k}{\partial y_j}$ by taking the derivative of the error.

    e.g., in the case of the squared error, we have $\frac{\partial E_k}{\partial y_j} = y_j - d_{kj}$.

MLP – Backpropagation

Input: A training set $D = \left\{ \left(\vec{x}_k, \vec{d}_k\right) \quad \middle| \quad k = 1, \ldots, p \right\}$ and the current vector of weights $\vec{w}$.

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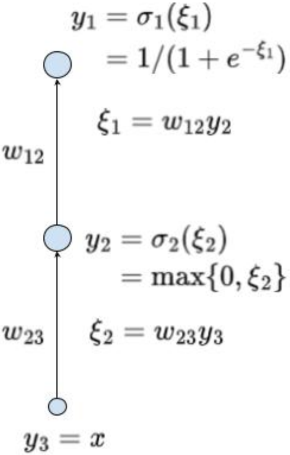
    e.g., in the case of the squared error, we have $\frac{\partial E_k}{\partial y_j} = y_j - d_{kj}$.
  - In the layer ℓ, assuming that $\frac{\partial E_k}{\partial y_r}$ has been computed for all neurons r in the layer $\ell + 1$, compute

    $$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot w_{rj}$$

    for all j from the ℓ-th layer. Here σ_r' is the derivative of σ_r.
  - Put $\frac{\partial E_k}{\partial w_{ji}} = \frac{\partial E_k}{\partial y_j} \cdot \sigma_j'(\xi_j) \cdot y_i$

Output: $\frac{\partial E}{\partial w_{ji}} = \sum_{k=1}^{p} \frac{\partial E_k}{\partial w_{ji}}$.

MLP Learning Example



Training set:

$$D = \{(x, d)\} = \{(1, 1)\}$$

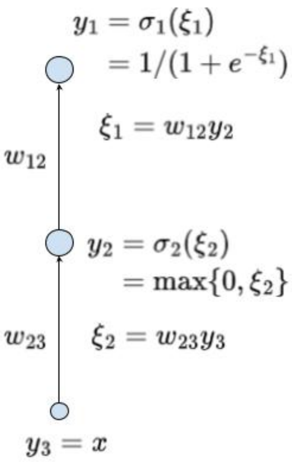
That is

$$y_3 = x = 1$$
$$d = 1$$

Error cross-entropy:

$$\begin{aligned} E(\vec{w}) &= -(d\log(y_1) + (1-d)\log(1-y_1)) \\ &= -\log(y_1) \end{aligned}$$

MLP Learning Example



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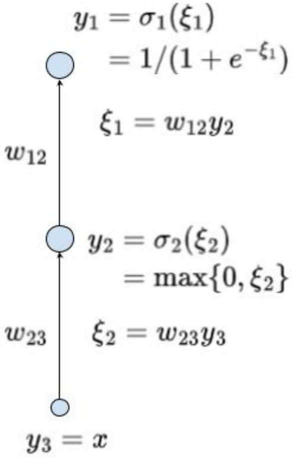
Error cross-entropy:

$$E(\vec{w}) = -(d \log(y_1) + (1-d)\log(1-y_1)) = -\log(y_1)$$

Assume the initial weight vector $\vec{w}^{(0)} = (w_{12}^{(0)}, w_{23}^{(0)}) = (\frac{1}{4}, 2)$.

Consider the learning rate $\varepsilon = 0.5$.

MLP Learning Example – Gradient Descent



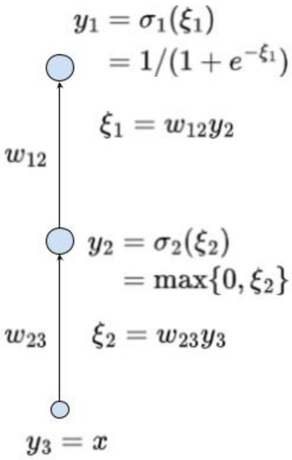
To make the gradient descent step:

$$w_{12}^{(1)} = w_{12}^{(0)} - \varepsilon \frac{\partial E}{\partial w_{12}}(\vec{w}^{(0)})$$

$$w_{23}^{(1)} = w_{23}^{(0)} - \varepsilon \frac{\partial E}{\partial w_{23}}(\vec{w}^{(0)})$$

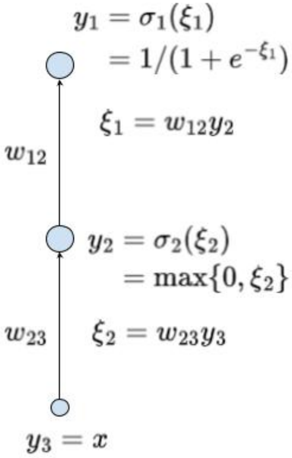
we need to compute the partial derivatives $\frac{\partial E}{\partial w_{12}}$ and $\frac{\partial E}{\partial w_{23}}$.

MLP Learning Example – Forward Pass



We have $x = 1, w_{12}^{(0)} = 1/4, w_{23}^{(0)} = 2$

MLP Learning Example – Forward Pass



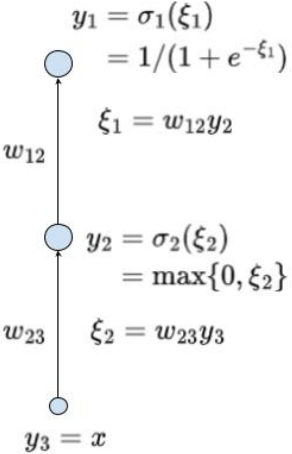
We have $x = 1, w_{12}^{(0)} = 1/4, w_{23}^{(0)} = 2$

First, compute the **forward pass**

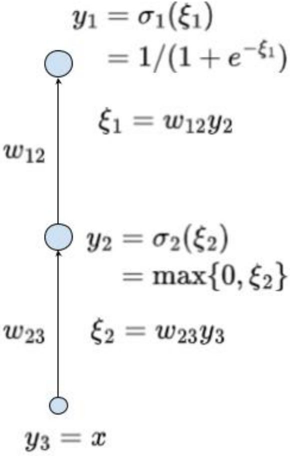
$$
\begin{aligned}
y_3 &= x = 1 \\
\xi_2 &= w_{23}^{(0)} y_3 = 2y_3 = 2 \\
y_2 &= \max\{0, \xi_2\} = 2 \\
\xi_1 &= w_{12}^{(0)} y_2 = \frac{1}{4} 2 = \frac{1}{2} \\
y_1 &= 1/(1+e^{-\xi_1}) = 1/(1+e^{-(1/2)}) \\
&= 0.6225
\end{aligned}
$$

MLP Learning Example – Backward Pass

We have $w_{12}^{(0)} = 1/4, w_{23}^{(0)} = 2, y_1 = 0.6225, y_2 = 2, y_3 = 1.$



MLP Learning Example – Backward Pass

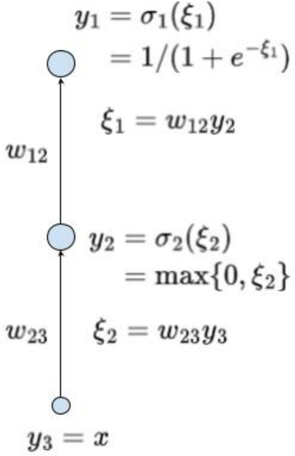


We have $w_{12}^{(0)} = 1/4, w_{23}^{(0)} = 2, y_1 = 0.6225, y_2 = 2, y_3 = 1$.

Proceed with the backward pass:

$$\frac{\partial E}{\partial y_1} = \frac{\partial(-\log(y_1))}{\partial y_1} = -\frac{1}{y_1} = -1.6065$$

MLP Learning Example – Backward Pass



We have $w_{12}^{(0)} = 1/4$, $w_{23}^{(0)} = 2$, $y_1 = 0.6225$, $y_2 = 2$, $y_3 = 1$.

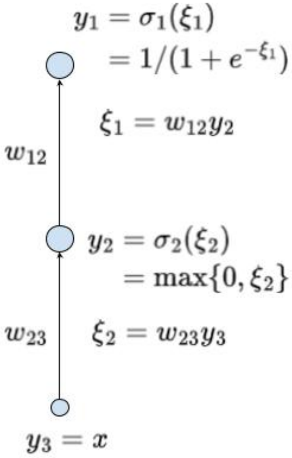
Proceed with the backward pass:

$$\frac{\partial E}{\partial y_1} = \frac{\partial(-\log(y_1))}{\partial y_1} = -\frac{1}{y_1} = -1.6065$$

Since $\sigma_1' = \sigma_1(1 - \sigma_1)$

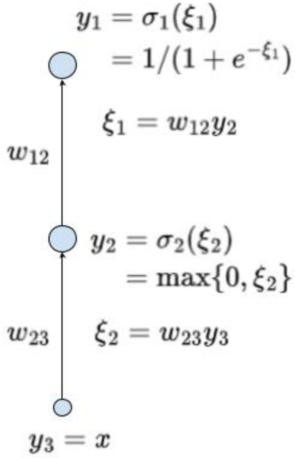
$$\begin{aligned}
\frac{\partial E}{\partial y_2} &= \frac{\partial E}{\partial y_1}\sigma_1'(\xi_1)w_{12}^{(0)} \\
&= \frac{\partial E}{\partial y_1}\sigma_1(\xi_1)(1 - \sigma_1(\xi_1))w_{12}^{(0)} \\
&= \frac{\partial E}{\partial y_1}y_1(1 - y_1)w_{12}^{(0)} \\
&= -1.6065 \cdot 0.6225 \cdot 0.3775 \cdot (1/4) \\
&= -0.09438
\end{aligned}$$

MLP Learning Example – The Gradient



We have
$w_{12}^{(0)} = 1/4, w_{23}^{(0)} = 2, y_1 = 0.6225, y_2 = 2, y_3 = 1, \frac{\partial E}{\partial y_1} = -1.6065, \frac{\partial E}{\partial y_2} = -0.09438.$

MLP Learning Example – The Gradient

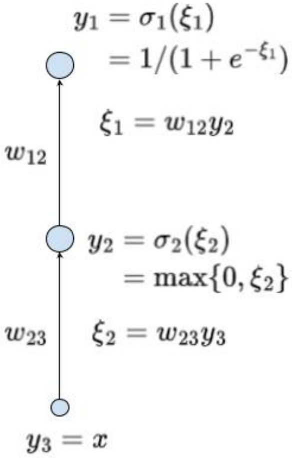


We have
$w_{12}^{(0)} = 1/4, w_{23}^{(0)} = 2, y_1 = 0.6225, y_2 = 2, y_3 = 1, \frac{\partial E}{\partial y_1} = -1.6065, \frac{\partial E}{\partial y_2} = -0.09438.$

Compute derivatives of E w.r.t. weights:

$$\begin{aligned}\frac{\partial E}{\partial w_{12}} &= \frac{\partial E}{\partial y_1}\sigma_1'(\xi_1) y_2 \\ &= \frac{\partial E}{\partial y_1} y_1(1-y_1) y_2 \\ &= -0.755\end{aligned}$$

MLP Learning Example – The Gradient



We have
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Compute derivatives of E w.r.t. weights:

$$\frac{\partial E}{\partial w_{12}} = \frac{\partial E}{\partial y_1}\sigma_1'(\xi_1)y_2 = \frac{\partial E}{\partial y_1}y_1(1-y_1)y_2 = -0.755$$

$$\frac{\partial E}{\partial w_{23}} = \frac{\partial E}{\partial y_2}\sigma_2'(\xi_2)y_3 = \frac{\partial E}{\partial y_2}y_3 = -0.09438$$

Backpropagation – Example – Summary

Forward pass (bottom up)

$$y_1 = \sigma_1(\xi_1) = 1/(1+e^{-\xi_1}) = 0.6225$$

$$w_{12}^{(0)} = 1/4 \qquad \xi_1 = w_{12}^{(0)} y_2 = 1/2$$

$$y_2 = \sigma_2(\xi_2) = \max\{0, \xi_2\} = 2$$

$$w_{23}^{(0)} = 2 \qquad \xi_2 = w_{23}^{(0)} y_3 = 2$$

$$y_3 = x = 1$$

Backpropagation – Example – Summary

Forward pass (bottom up)

$$y_1 = \sigma_1(\xi_1) = 1/(1+e^{-\xi_1}) = 0.6225$$

$$w_{12}^{(0)} = 1/4 \qquad \xi_1 = w_{12}^{(0)} y_2 = 1/2$$

$$y_2 = \sigma_2(\xi_2) = \max\{0, \xi_2\} = 2$$

$$w_{23}^{(0)} = 2 \qquad \xi_2 = w_{23}^{(0)} y_3 = 2$$

$$y_3 = x = 1$$

Backward pass (top down)

$$\frac{\partial E}{\partial y_1} = 1/y_1 = -1.6065$$

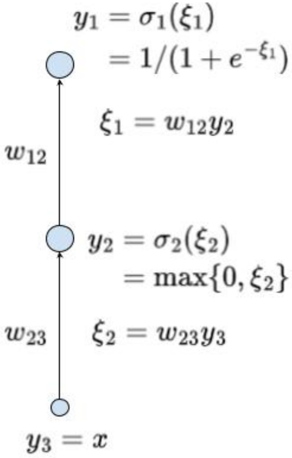
$$\frac{\partial E}{\partial w_{12}} = \frac{\partial E}{\partial y_1} y_1(1-y_1)y_2 = -0.755$$

$$\frac{\partial E}{\partial y_2} = \frac{\partial E}{\partial y_1} y_1(1-y_1)w_{12}^{(0)} = -0.09438$$

$$\frac{\partial E}{\partial w_{23}} = \frac{\partial E}{\partial y_2} 1 y_3 = -0.09438$$

Note that **WE HAVE NOT YET CHANGED ANY WEIGHTS!**

MLP Learning Example – Gradient Descent Step



So **ONLY NOW** we can make the **learning step** and change the weights:

$$w_{12}^{(1)} = w_{12}^{(0)} - \varepsilon \frac{\partial E}{\partial w_{12}}(\vec{w}^{(0)}) = \frac{1}{4} - 0.5 \cdot (-0.755) = 0.627$$

$$w_{23}^{(1)} = w_{23}^{(0)} - \varepsilon \frac{\partial E}{\partial w_{23}}(\vec{w}^{(0)}) = 2 - 0.5 \cdot (-0.09438) = 2.047$$

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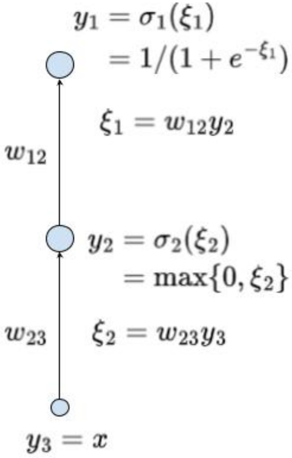

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We have made just a **single** gradient descent step!

MLP Training Summary

- MLP are trained using the **gradient descent** algorithm

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- Training of neural networks in practice is tricky due to many reasons comprising in particular
  - highly complex non-linear shape of the error function,
  - tendency to overfit very quickly,
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An advice: Always concentrate the main effort on the solved problem formulation and, afterward, on the data you have at your disposal (and honestly separate the Test set right at the beginning).

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- In 2006, a solution was found by Hinton et al.:
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    More precisely: The lowest hidden layer learns patterns in data, the second lowest learns patterns in data transformed through the first layer, and so on.

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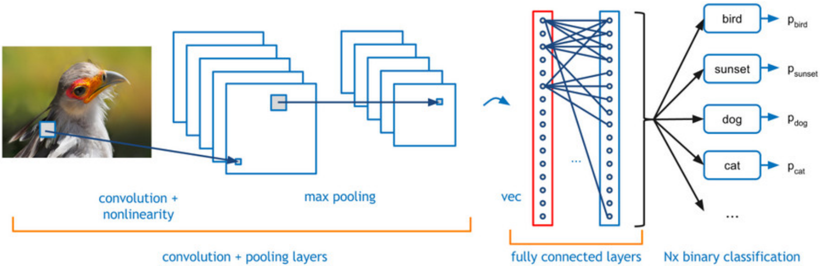
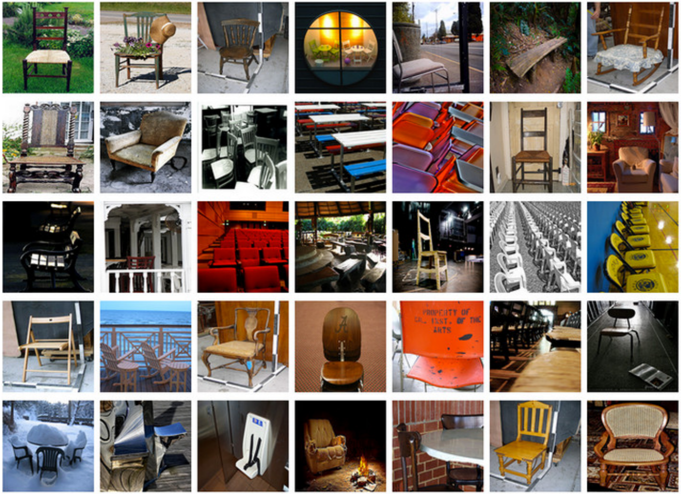
  - Then use a supervised learning algorithm to only *fine tune* the weights to the desired input-output behavior.
- ... but the actual revolution started with convolutional networks trained on several GPUs.

Convolutional network



ImageNet Large-Scale Visual Recognition Challenge (ILSVRC)

ImageNet database (16,000,000 color images, 20,000 categories)



ImageNet Large-Scale Visual Recognition Challenge (ILSVRC)

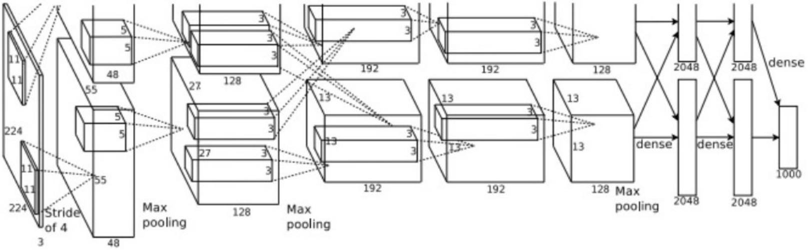
Competition in classification over a subset of images from ImageNet.

In 2012, training saw 1,200,000 images and 1000 categories. Validation set 50,000, Test set 150,000.

Many images contain several objects $\rightarrow$ typical rule is top-5 highest probability assigned by the net.

KSH net

ImageNet classification with deep convolutional neural networks, by Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton (2012).



Trained on two GPUs (NVIDIA GeForce GTX 580)

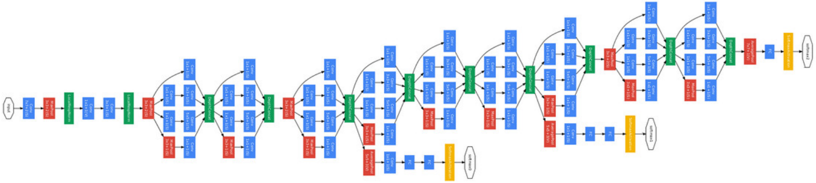
Results:

- Accuracy 84.7% in top-5 (second best alg. at the time: 73.8%)
- 63.3% in "perfect" classification (top-1)

ILSVRC 2014

The same set of images as in 2012, top-5 criterium.

GoogLeNet: deep convolutional net, 22 layers



Results:

- 93.33% in top-5

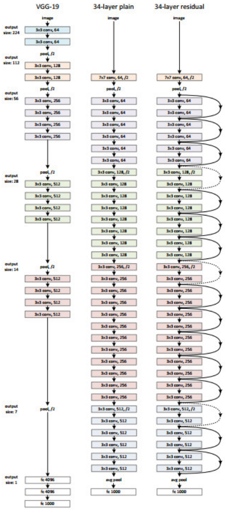
Superhuman power?

Superhuman GoogLeNet?!

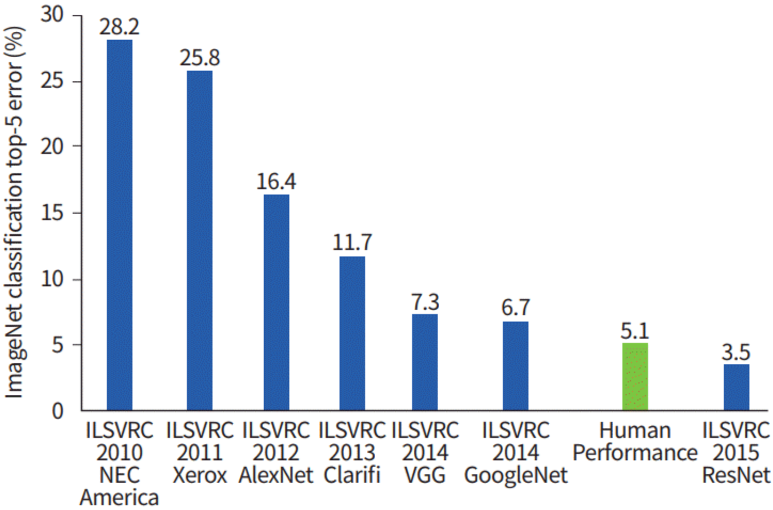
Andrej Karpathy: ...the task of labeling images with 5 out of 1000 categories quickly turned out to be highly challenging, even for some friends in the lab who have been working on ILSVRC and its classes for a while. First, we thought we would put it up on [Amazon Mechanical Turk]. Then, we thought we could recruit paid undergrads. Then, I organized a labeling party of intense labeling effort only among the (expert labelers) in our lab. Then, I developed a modified interface that used GoogLeNet predictions to prune the number of categories from 1000 to only about 100. It was still too hard - people kept missing categories and getting up to ranges of 13-15% error rates. In the end, I realized that to get anywhere competitively close to GoogLeNet, it would be most efficient if I sat down and went through the painfully long training process and the subsequent careful annotation process myself. The labeling happened at a rate of about 1 per minute, but this decreased over time... Some images are easily recognized, while some pictures (such as those of fine-grained breeds of dogs, birds, or monkeys) can require multiple minutes of concentrated effort. I became very good at identifying breeds of dogs... Based on the sample of images I worked on, the GoogLeNet classification error turned out to be 6.8%... In the end, my error turned out to be 5.1%

ILSVRC 2015

- Microsoft network ResNet: 152 layers, complex architecture
- Trained on 8 GPUs
- 96.43% **accuracy** in top-5



ILSVRC



ImageNet classification top-5 error (%)
30
25
20
15
10
5
0
28.2
25.8
16.4
11.7
7.3
6.7
5.1
3.5
ILSVRC 2010 NEC America
ILSVRC 2011 Xerox
ILSVRC 2012 AlexNet
ILSVRC 2013 Clarifi
ILSVRC 2014 VGG
ILSVRC 2014 GoogleNet
Human Performance
ILSVRC 2015 ResNet

ILSVRC 2016

Trumps-Soushen (The Third Research Institute of Ministry of Public Security)

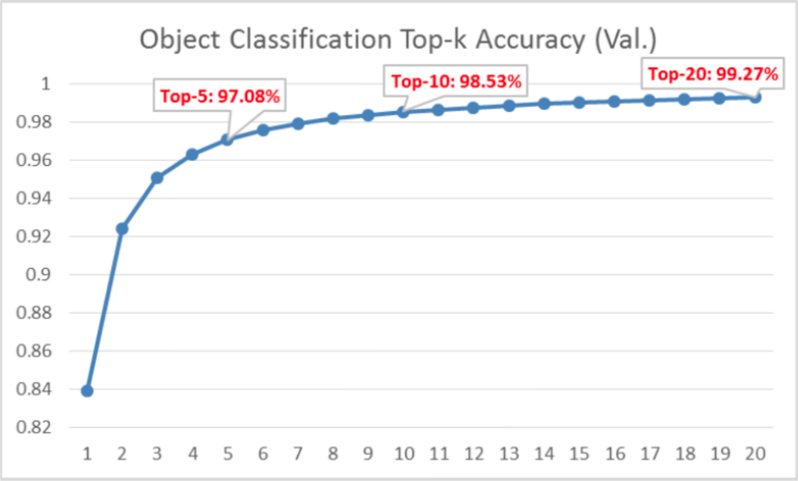
There is no new innovative technology or novelty by Trimps-Soushen.

Ensemble of the pre-trained models from previous years.

Each model is strong at classifying some categories but weak at categorizing others.

Test error: 2.99%

Top-k accuracy analyzed



https://towardsdatascience.com/review-trimps-soushen-winner-in-ilsvrc-2016-image-classification-dfbc423111dd

Top-20 typical errors

Out of 1458 misclassified images in Top-20:

Error Categories	Numbers	Percentages(%)
Label May Wrong	221	15.16
Multiple Objects (>5)	118	8.09
Non-Obvious Main Object	355	24.35
Confusing Label	206	14.13
Fine-grained Label	258	17.70
Obvious Wrong	234	16.05
Partial Object	66	4.53

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Top-k accuracy analyzed

Predict:
1 *pencil box*
2 *diaper*
3 *bib*
4 *purse*
5 *running shoe*

Ground Truth:
sleeping bag

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Top-k accuracy analyzed

Predict:
1 *dock*
2 *submarine*
3 *boathouse*
4 *breakwater*
5 *lifeboat*

Ground Truth:
paper towel

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Top-k accuracy analyzed

Predict:
1 *bolete*
2 *earthstar*
3 *gyromitra*
4 *hen of the woods*
5 *mushroom*

Ground Truth:
stinkhorn

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Top-k accuracy analyzed

Predict:
1 *apron*
2 *plastic bag*
3 *sleeping bag*
4 *umbrella*
5 *bulletproof vest*

Ground Truth:
poncho

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