
# Machine Learning

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# Agenda

- Machine learning Introduction
  - Supervised learning
  - Unsupervised learning
  - Machine Learning in Bioinformatics

- Supervised learning
  - Workflow
  - Overfitting
  - Feature selection
  - Classifier evaluation and comparison
  - Algorithms
    - Naïve Bayes
    - Instance-based
    - Decision trees
    - Linear

# Machine Learning Introduction

# What is Machine Learning?

Trying to make machines able to solve problems without explicitly programming them

**"Training" instead of programming**

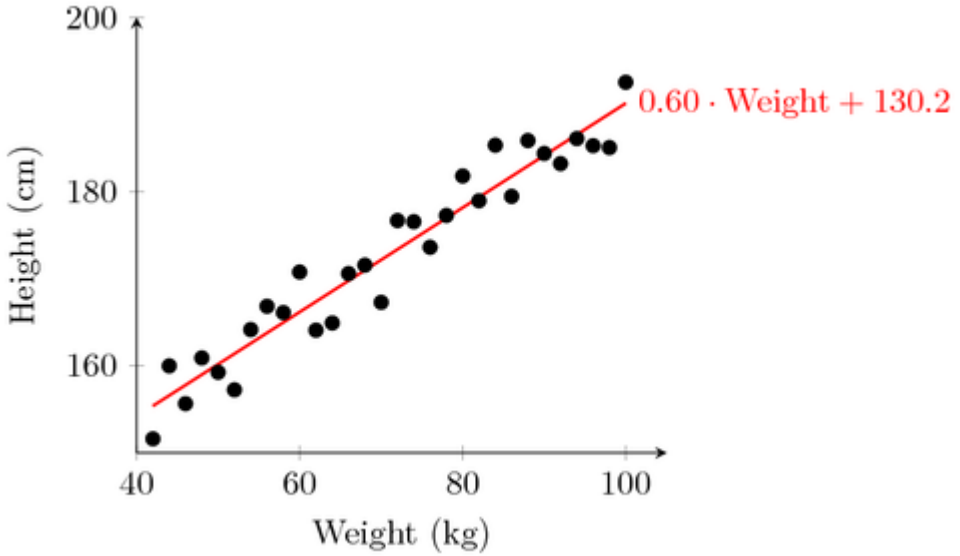
Types

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

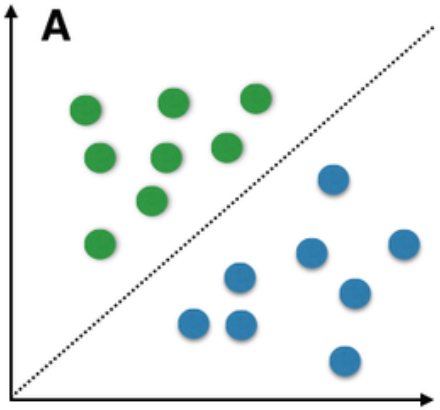
# Supervised learning

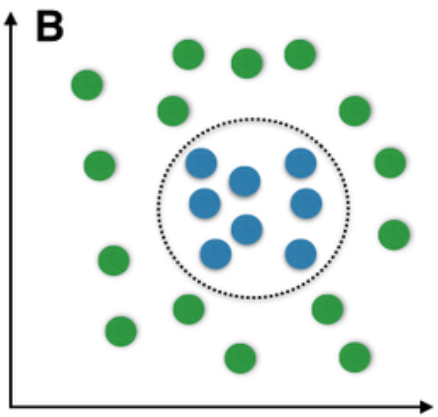
*Given a set of "instances", each one with a set of measured "attributes" and an "outcome" value, we want to train a "model", that predicts the outcome in further problem instances.*

Regression (outcome is a number)



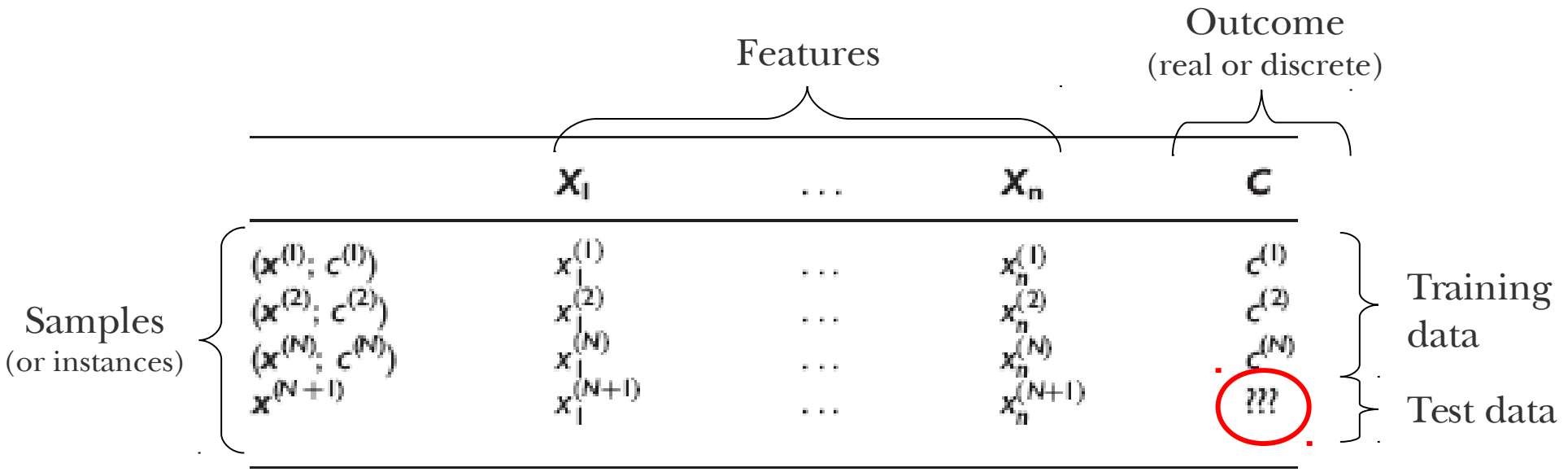

Classification (outcome is a category)



# Supervised learning

## Input dataset structure for learning



# Supervised learning

## Popular techniques

### Bayesian classifiers:

Naive Bayes, semi-NB, Tree augmented NB, k dependence Bayesian…

### Classification trees:

CART, C4.5, RandomForest, J48…

### K-Nearest Neighbours

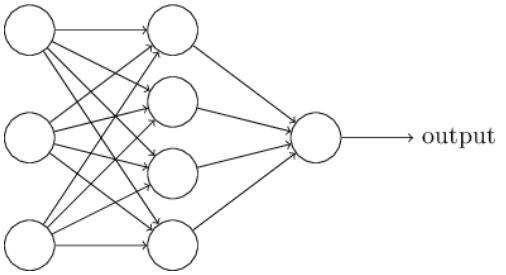
### Linear/Logistic regression

### Support Vector Machines

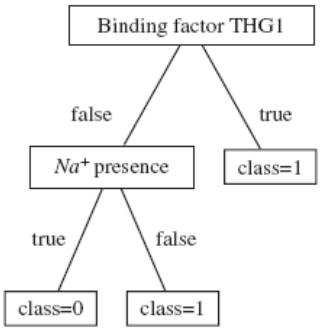
### Neural networks

### Meta: Bagging, Boosting

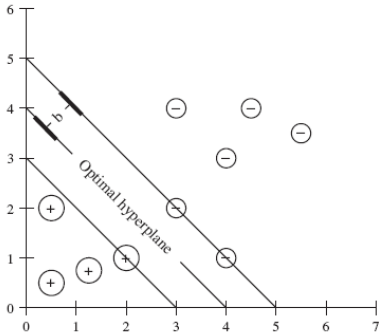
Neural Network

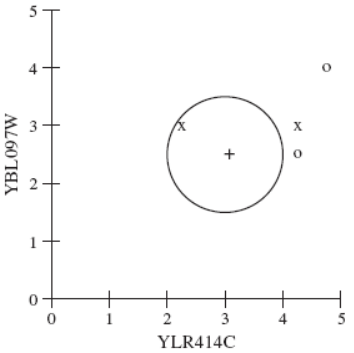



Classification Tree




Support Vector Machine




kNN classifier

# Unsupervised learning

*Learning underlying structures in data*

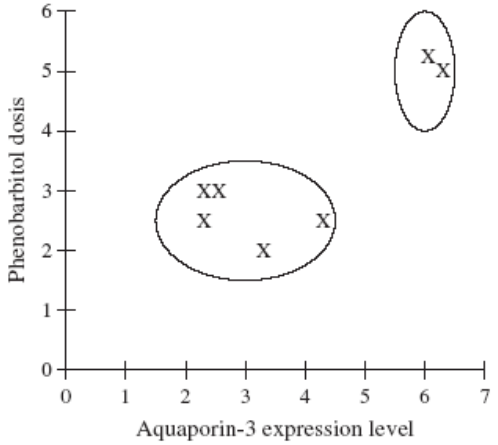
- Clustering (learn group of samples)
  - Partition a set of "instances" in several groups (clusters) given the differences between them
    - Their are based on "distances" between instances that is a problem-dependant issue
      - Typical: Euclidean, Pearson, Sperman
- Dimensionality reduction (learn alternative representations)
  - Reduce the number of input variables while trying to keep the maximum information of the dataset
    - Very useful for visualization ($n$ dimensions → 2D or 3D)

# Unsupervised learning

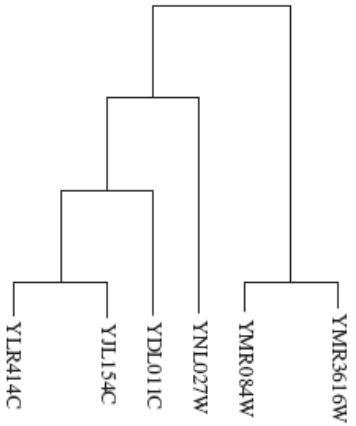
## Popular techniques

- Partition clustering
  - k-means, SOM, GCS, PAM
- Hierarchical clustering with single-linkage, complete linkage, centroid linkage and wards-criterion
  - They produce the popular “dendograms”
- Model-based clustering

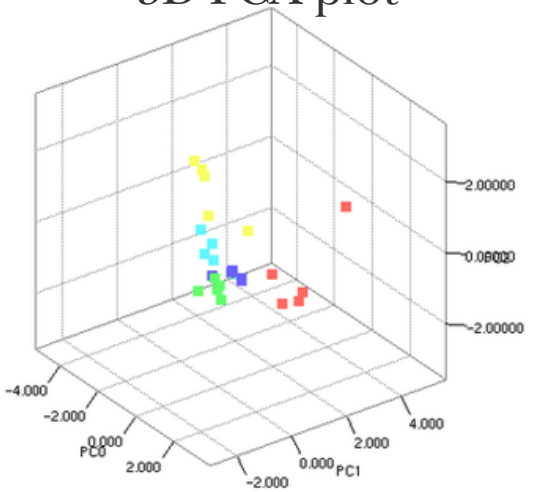
k-means




Hierarchical clustering




3D PCA plot



# Bioinformatics

*Application of the Information Technologies to the field of Molecular Biology*

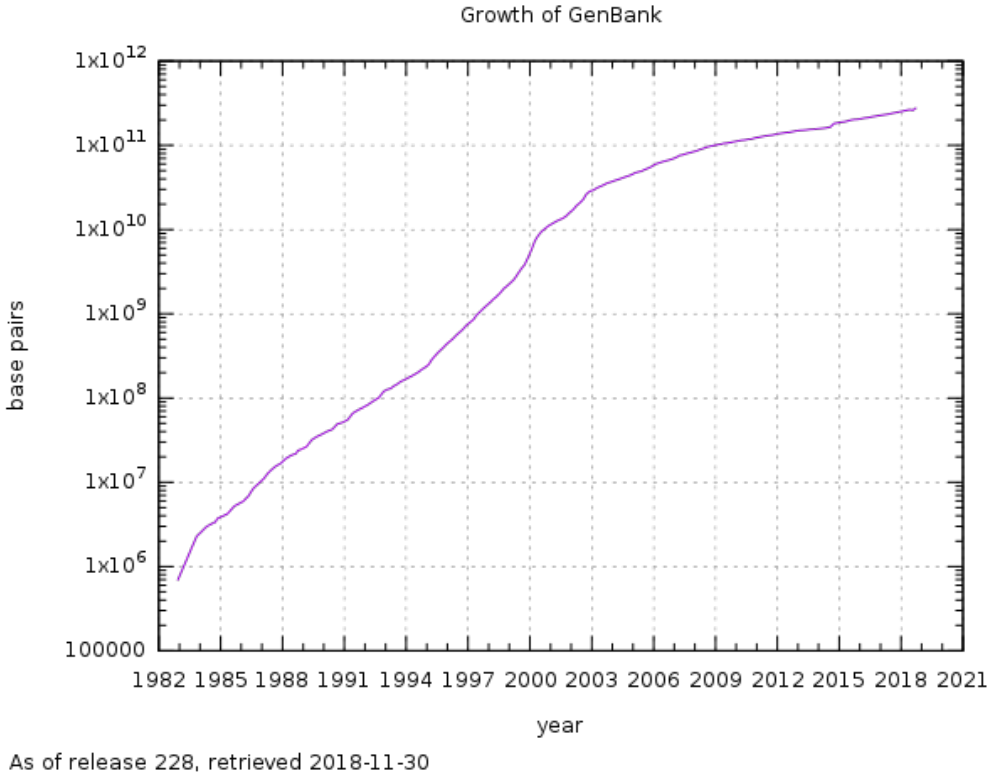
Databases

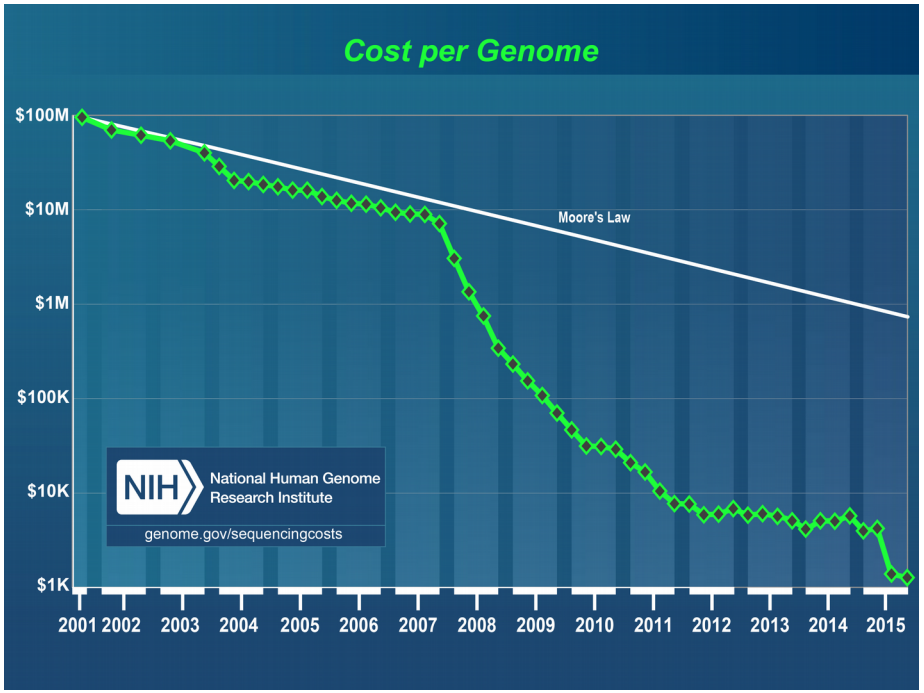
Algorithms

Statistical techniques

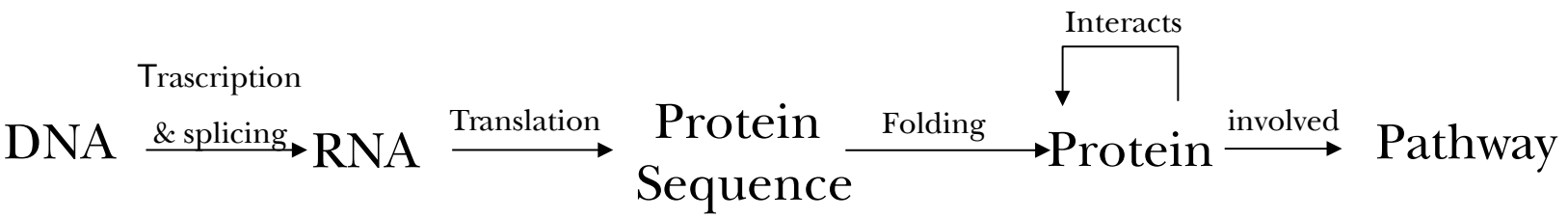
*… to solve formal and practical problems arising from the management and analysis of biological data*

# Bioinformatics



# *The Dogma* & Bioinformatics




| Nucleotide sequence | Transcripts | Aminoacid sequence | 3D structure | Set of Reactions |
|---|---|---|---|---|
| ACTTGTC<br>ATGGCGA<br>CTGTCCT<br>TTGTGC<br>… | | MEEPQSDPSV<br>EPPLSQETFSD<br>LWKLLPENNV<br>LS… | | |

Interactomics

| GENOMICS | PROTEOMICS | METABOLOMICS |
|---|---|---|
| Sequence analysis<br><br>Genome annotation<br><br>Analysis of mutations [DNA-seq]<br><br>Gene expression analysis [microarrays/RNA-seq]<br><br>**Evolution**<br>Phylogenetic reconstruction<br>Comparative genomics | Protein expression analysis [mass spectometry]<br><br>Protein interaction prediction [3D docking]<br><br>Protein structure prediction [folding] | Modelling biological systems<br>Functional analysis |

# Bioinformatics Data

## Genomics

### Sequences

Entrez Nucleotide

EMBL NUCLEOTIDE SEQUENCE DATABASE

DDBJ DNA Data Bank of Japan

### Genomes

Entrez Genome

e! Ensembl

UCSC

TIGR

### Gene-centric

Entrez Gene

GeneCards®

## Proteomics

### Proteins

swissprot

TrEMBL TRANSLATED EMBL

Entrez Protein

UniProt the universal protein resource

PIR

### Structure

PDB PROTEIN DATA BANK

SCOP STRUCTURAL CLASSIFICATION OF PROTEINS

CATH Protein Structure Classification

### Domains

prosite

InterPro

Conserved Domains

Pfam

SMART

## Interactomics & Metabolomics

### Prot-Prot interactions

STRING

IntAct

### Pathways

KEGG

BIOCARTA

PathwayInteractionDatabase

GenMAPP Gene Map Annotator and Pathway Profiler

## Ontologies

the Gene Ontology

MeSH

## Bibliome

PubMed

## Experimental data

GEO Gene Expression Omnibus

ArrayExpress

# Supervised learn. in Bioinformatics


- Genomics
  - Gene finding (if a sequence is a coding region)
  - Splice site prediction (if a sequence is a splice site)
  - Predict disease genes (e.g: from its sequence length)
  - Prediction of mutation (SNP) effect
  - Cancer prediction from gene expression (microarrays/RNA-seq)
- Proteomics
  - Prediction of secondary structure (alpha-helix, beta-sheet, etc.)
  - Prediction of sub-cellular location of the protein
  - Cancer prediction from protein expression (mass spectra)

# Supervised learn. in Bioinformatics

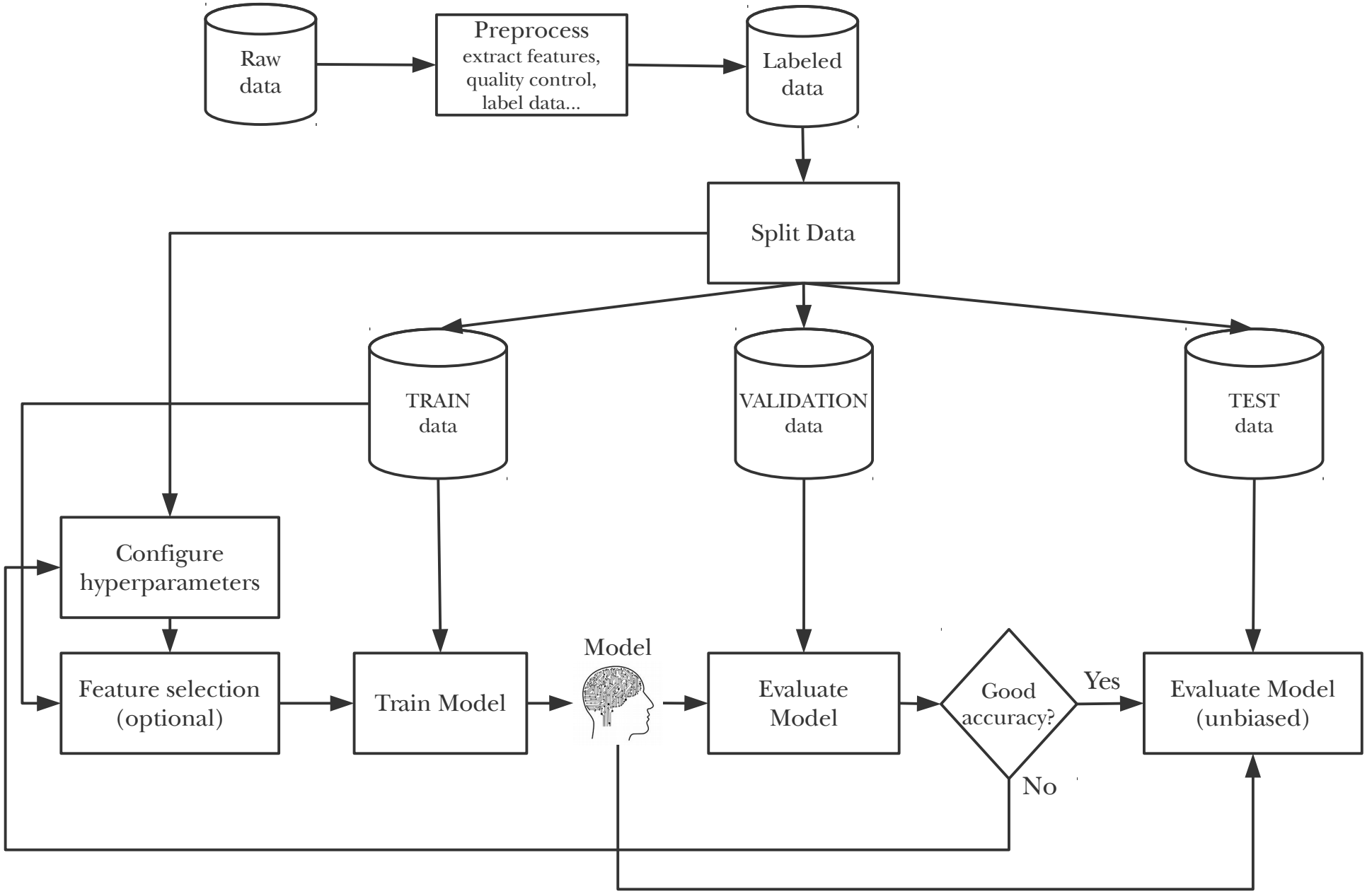
- Systems biology
  - Predict the cell migration speed (high, low) from the phosphorilation levels of signaling proteins
  - Predict a gene regulatory level (up-regulated or down-regulated given the 'related' genes expression)
- Text mining
  - Protein/gene recognition in biomedical literature
    - is this word a gene/protein given some word features: ortographic, part-of-speech, suffix, trigger words, etc…??

# Unsupervised learn. in Bioinformatics

- Mainly in Genomics and Proteomics
  - Co-expression detection (group of genes/proteins with similar expression)
  - Subclass discovery (group of samples given the expression of its genes)
  - Expression data visualization with dendograms

# Supervised Learning

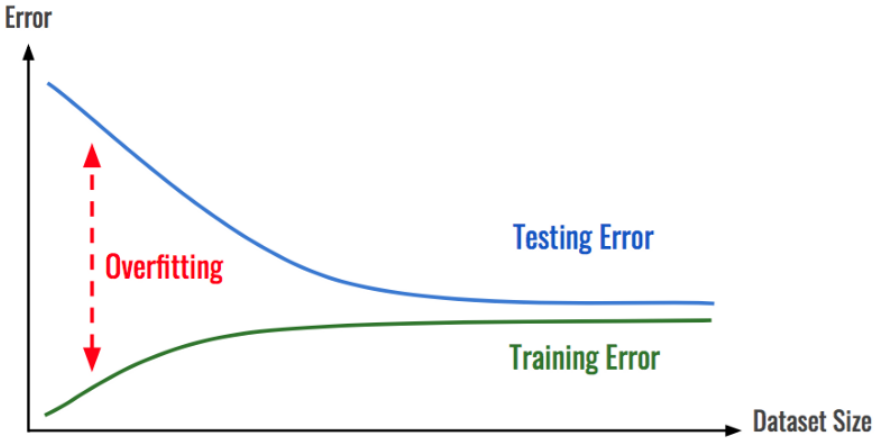
# Supervised learning workflow

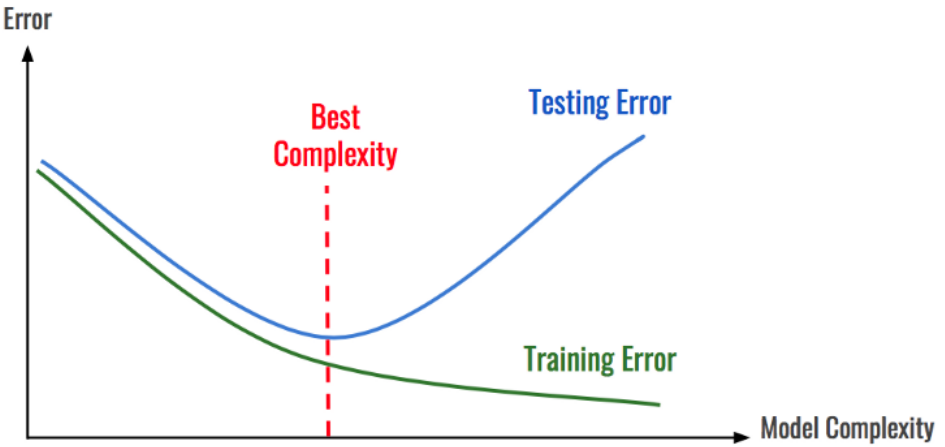


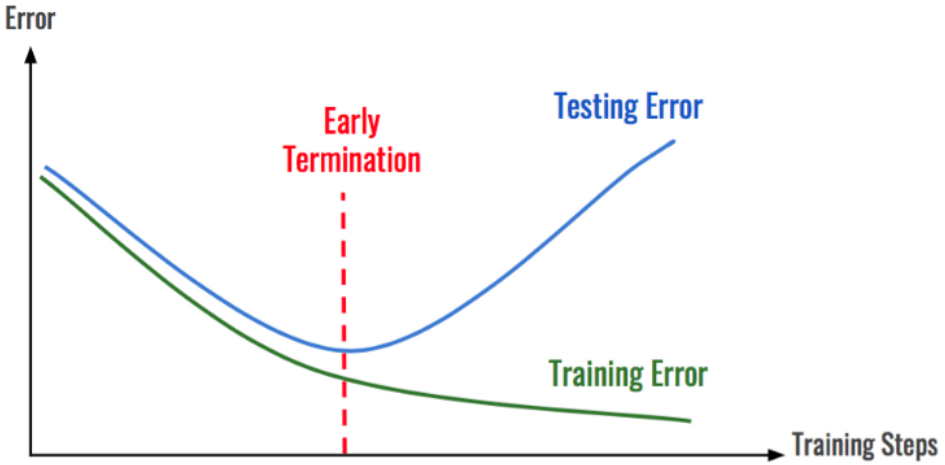
# Overfitting


https://hackernoon.com/memorizing-is-not-learning-6-tricks-to-prevent-overfitting-in-machine-learning-820b091dc42

# Overfitting




https://hackernoon.com/memorizing-is-not-learning-6-tricks-to-prevent-overfitting-in-machine-learning-820b091dc42

# Feature selection

Are all input attributes useful?

Advantages: reduced cost in data acquisition, more interpretable models, faster training, and better accuracy

It is a search space problem ($2^n$-1), in general:

1. Generate a subset
   - Brute force (all possible subsets)
   - Deterministic/not deterministic heuristic search
2. Evaluate subset
   - Statistical estimation: Information Gain, X2, t-test, DFP, CFS
   - Wrapper (use classifier accuracy in training set)
3. if (!halt_condition) GOTO 1

# Classifier evaluation and comparison

# Classifier evaluation

## Performance metrics. In binary classification:

| Predicted \ Actual | Positive | Negative | |
|---|---|---|---|
| Positive | True Positives (TP) | False Positives (FP)<br>Type-I error | Positive Predictive Value (PPV) or precision<br>= TP / (TP + FP)<br><br>False Discovery Rate (FDR) = 1 - PPV |
| Negative | False Negatives (FN)<br>Type-II error | True Negatives (TN) | Negative Predictive Value (NPV)<br>= TN / (FN + TN)<br><br>False Omission Rate (FOR) = 1 - NPV |
| | Sensitivity or recall or True positive rate (TPR) =<br>TP / (TP+FN)<br><br>False Negative Rate (FNR)<br>= 1 - TPR | Specificity or True Negative Rate (TNR)<br>=<br>TN / (FP+TN)<br><br>False Positive Rate (FPR)<br>= 1 - TNR | Accuracy = (TP + TN) / N |

# Classifier evaluation

Performance metrics. In multi-class classification:

Accuracy and kappa are valid for multi-class classifier evaluation

We can also use the previous metrics for each class by considering

positive = class

negative = other classes

However, there will be multiple sensitivities, specificities, PPV, etc. (one per class)

# Classifier evaluation

Ideally, we should do several tests for a model in order to better estimate its real performance. If the test data is big enough, and not biased, the estimation is good

However, when we have a reduced number of samples, it is not easy. There are several validation frameworks:

- Holdout
- Bootstrapping
- Cross-validation

# Classifier evaluation

## Holdout

- Divide dataset randomly in several subsets
- In general, we take 2/3 for train and the rest for test
- Variant: “resampling”
  - It consists in conducing several holdout test over different train and test datasets

# Classifier evaluation

## Bootstrapping

Given a dataset with N samples

Create a training set of size N, taking samples N times randomly, with replacement

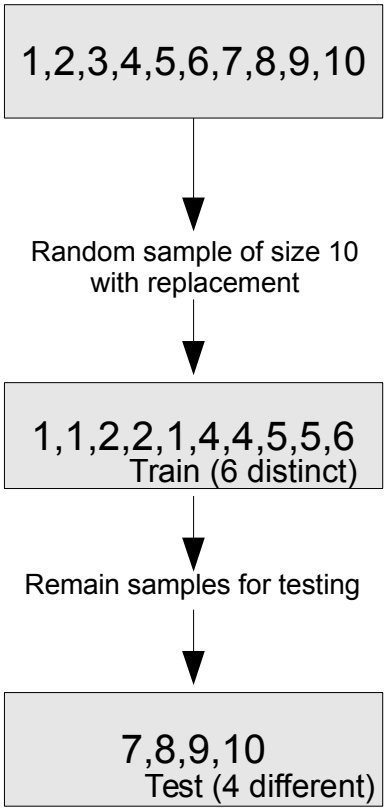
In general, with a size big enough, the number of different instances in the sample tends towards 63.2% of N

$$P(\text{of being selected with 1 trial}) = \frac{1}{N}$$

$$P(\text{not being selected}) = 1 - \frac{1}{N}$$

$$P(\text{not being selected in N trials}) = \left(1 - \frac{1}{N}\right)^n \approx e^{-1} = 0.368$$

$$\text{Number of different samples on train} = 1 - 0.368 = 0.632$$




The final error of this method can be weighted using the training error:

$$e = 0.632 \cdot e_{\text{test}} + 0.368 \cdot e_{\text{train}}$$

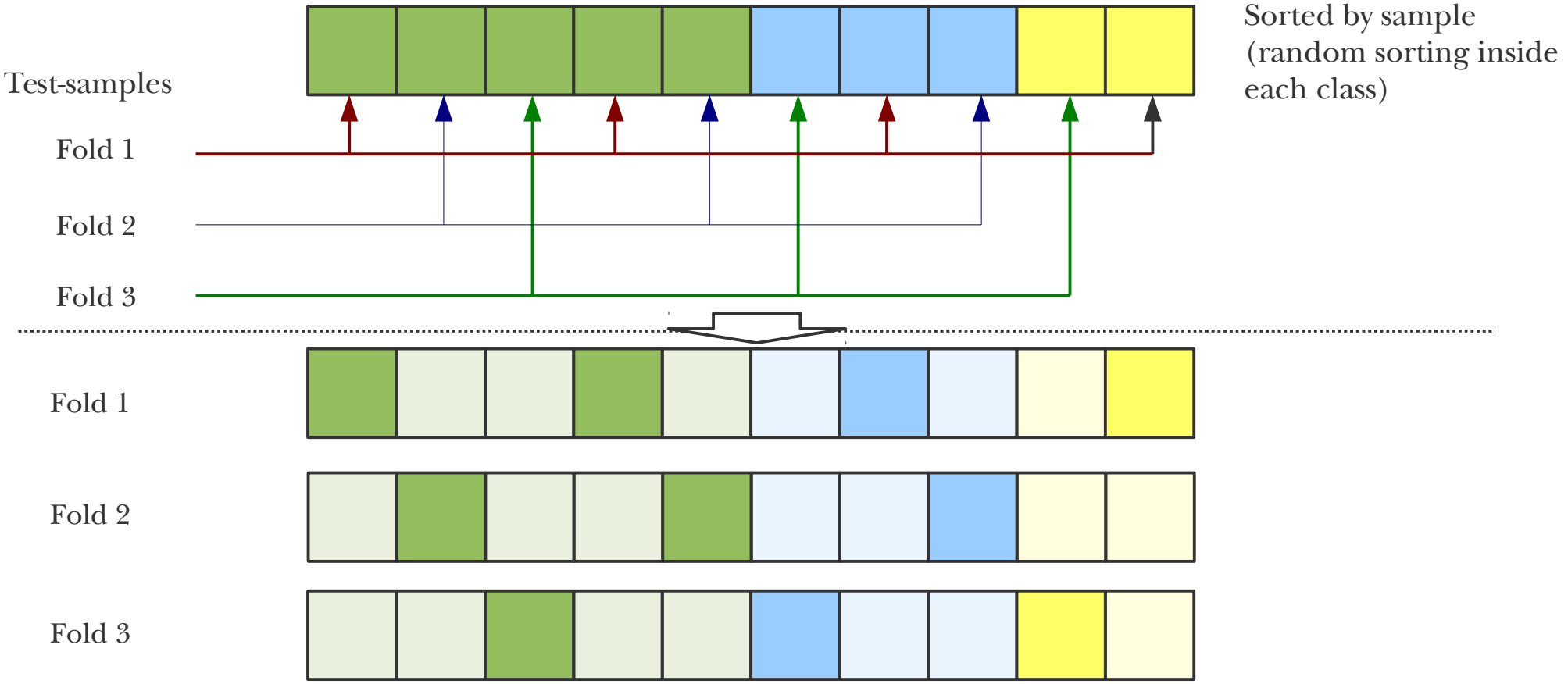
# Classifier evaluation

- Cross-validation (CV)
  - Create K pairs of training and test
    - Example. With 10 samples, conduct a 3-fold CV, we get 3 pairs, with a 33% of samples for testing and the rest for training
  - Each sample appears as test sample in exactly one pair
  - K=10 is one of the most popular value
  - To better estimate the performance, we can repeat CV 10 times, giving a total of 100 train-test experiments
  - Stratified: keep the same class distribution of the complete dataset in each train/test subsamples
  - Leave-one-out. Variant where K=N, that is, the test subset in each pair has only one sample
    - Useful when there are very few training samples

# Classifier evaluation

## Cross validation.

### Example. Stratified 3-fold CV



# Classifier comparison

- We can use the CV error directly
  - However, differences can be due to chance
  - We can employ statistical tests over CV estimations to tell if differences are statistically significant. Example methods
    - McNemar test
    - CV + Paired t-test
    - 5x 2-fold-CV + Paired t-test
    - Repeated CVs + corrected resampled t-test (weka)

# Classifier comparison

## McNemar test

Given the output of two classifiers (A,B) for each sample, we have 4 possibilities:

| | |
|---|---|
| $n_{00}$: Both classifiers fail | **$n_{01}$: A fails, B hits** |
| **$n_{10}$: B fails, A hits** | $n_{11}$: Both classifiers hit |

The next T score is based on observing differences between off-diagonal values ($n_{10}$ y $n_{01}$), which are cells counting when classifiers differ.

**Null hypothesis**. Differences between $n_{10}$ and $n_{01}$ is 0.

$$T = \frac{(|n_{01} - n_{10}| - 1)^2}{n_{01} + n_{10}}$$

This score follows a chi-squared distribution with 1 degree of freedom. For example a $T > 3.8414$ gives p-values $< 0.05$.

# Classifier comparison

CV + Paired t-test

Conduct a K-fold CV. We get K accuracies of each classifier

| | Fold 1 | Fold 2 | Fold 3 | Fold 4 | ... | Fold K |
|---|---|---|---|---|---|---|
| Classifier A | 0.7 | 0.75 | 0.78 | 0.79 | | 0.77 |
| Classifier B | 0.6 | 0.65 | 0.64 | 0.62 | | 0.69 |

Null hypothesis: both classifiers has the same mean accuracy

Conduct a Student's paired t-test

Problem: The t-test assumes independency of each pair
However, CV generates overlapping training samples

# Classifier comparison

## 5x 2CV + Paired t-test

### Conduct 2-fold CV 5 times

The first replicate to estimate error; all replicates to estimate variance

### On each of the 5 experiments:

| | Fold 1 | Fold 2 |
|---|---|---|
| Classifier A | 0.7 | 0.75 |
| Classifier B | 0.6 | 0.65 |

$p^{(1)}$: differences of A and B errors in fold 1

$p^{(2)}$: differences of A and B errors in fold 2

$$s^2 = (p^{(1)} - \bar{p})^2 + (p^{(2)} - \bar{p})^2$$

### Compute an statistic that follows a distribution similar to Student's t with 5 degrees of freedom:

$$\tilde{t} = \frac{p_1^{(1)}}{\sqrt{\frac{1}{5}\sum_{i=1}^{5} s_i^2}}$$

$i$ = iteration

With t < 2.02 we get p-values < 0.05

# Classifier comparison

Repeated CVs + corrected resampled t-test

Test included in Weka Experimenter

Conduct CV several times:

For example: 10x10-fold CV

We get 100 accuracy values for each classifier

Use a variant of Student's t-test which takes into account that samples are not independent (samples are repeated in different train-test samples) and also avoid the bias introduced with the total number of trials

$$t = \frac{\bar{d}}{\sqrt{\left(\frac{1}{k} + \frac{n_2}{n_1}\right)\sigma_d^2}}$$

$\bar{d}$ : classifier A and B accuracy mean differences in each trieal (100 trials)
$k$ : number of trials, in a 10x10CV, k is 100
$n_1$ : ratio for train , $n_2$ : ratio for test. In a 10CV $n_1$ is 0.9 and $n_2$ is 0.1

This score follows a Student's t distribution with folds-1 degrees of freedom (9 for 10-fold CV)

# Supervised Learning Algorithms

# Bayesian

## Naïve Bayes

Classification consist in find P(class | features)

With conditional dependencies (using Bayes). We need to know $2^n$ different probabilities (n=number of features, unfeasible).

$$P(A|B)=\frac{P(B|A)P(A)}{P(B)} \qquad P(cavities|pain\wedge infection)=\frac{P(pain\wedge infection|cavities)P(cavities)}{P(pain\wedge infection)}$$

With **conditional independence**

Idea: two random variables can be independent once a third variable is known.

Mathematically:

$$P(pain\wedge infection|cavities)=P(pain|cavities)P(infection|cavities)$$

*pain* and *infection* are independent once the value of *cavities* is known

Replacing in the previous Bayes formula:

$$P(cavities|pain\wedge infection)=\frac{P(pain|cavities)P(infection|cavities)P(cavities)}{P(pain\wedge infection)}$$

$$P(\neg cavities|pain\wedge infection)=\frac{P(pain|\neg cavities)P(infection|\neg cavities)P(\neg cavities)}{P(pain\wedge infection)}$$

**Conditional indedepencence allows us to scale probability-based systems; indeed, they are more available than those assuming total independence**

# Bayesian

## Naïve Bayes

### Conditional independence (cont)

So we have:

effects(s)

$$P(C|F_1,\ldots,F_n) = \alpha P(C)\prod_{i=1}^{n} P(F_i|C)$$

cause

α=(1/denominator) in the Bayes function. It can be solved by considering that P(c) + P(¬c) = 1

It is a typical pattern: One cause has multiple effects, all of them conditionally independent, once such cause is known.

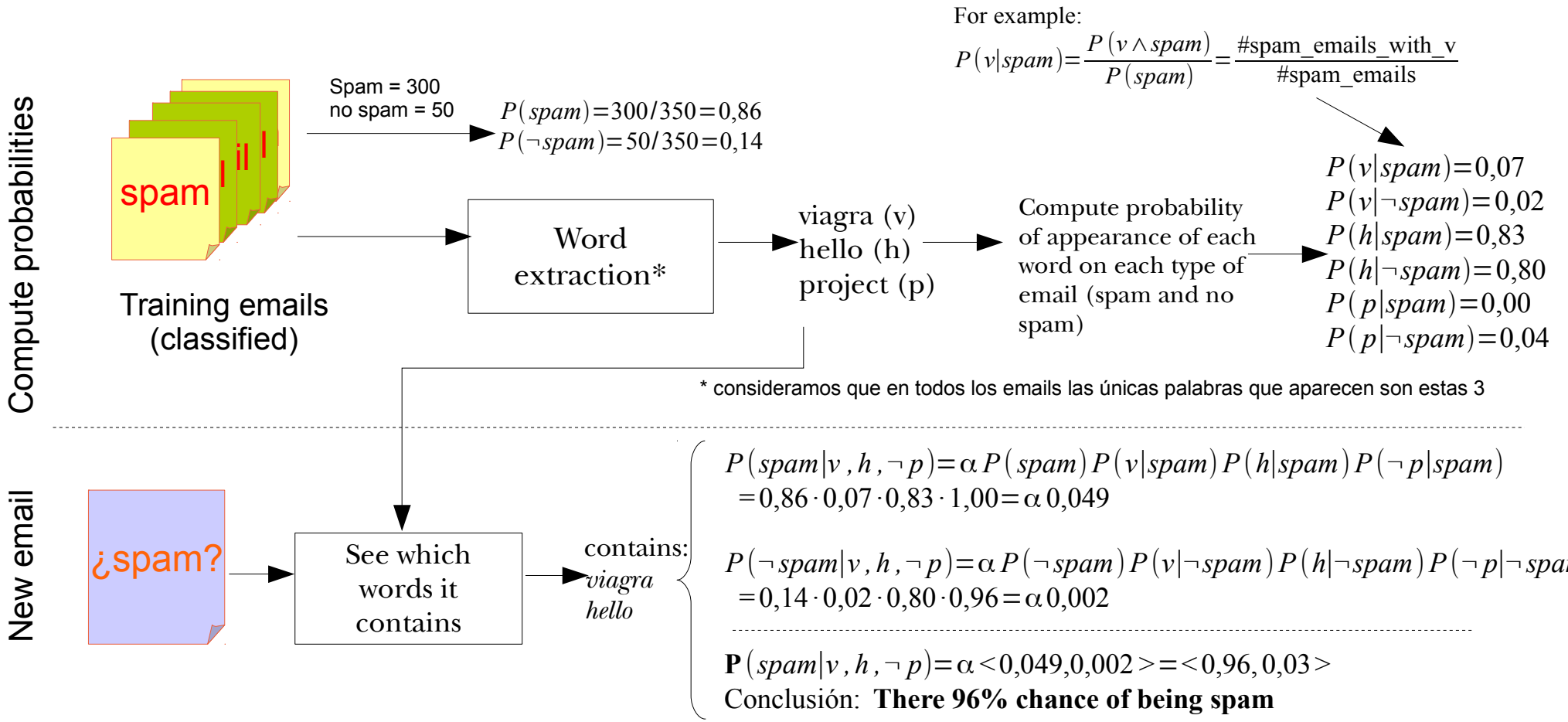
**Naïve-Bayes** (or simple-Bayes)

Sometimes, even when such conditional independence is not real, we make this assumption in order to make the system feasible

# Bayesian

## Naïve Bayes

### Naive-Bayes. Example: Detecting spam email



# Instance based

## Introduction

During training, we save all samples without any modification.

With a *distance function* we find the nearest saved sample to the new sample and we give the class of the found sample as prediction.

## Distance functions:

Euclidean $$dist(p,q)=\sqrt{\sum_{i=1}^{n}(p_i-q_i)^2}$$

Manhattan $$dist(p,q)=\sum_{i=1}^{n}|p_i-q_i|$$

Euclidean, with exponent >2 (increases the influence in greater distances).

# Instance based

## Normalization

If attributes have a different scale (for example, age [0, 100] and price [10k, 100k], attributes with larger values have bigger influence, so it is typical to normalize them, for example:

feature scaling:

$$scale(v_i) = \frac{v_i - min\, v_i}{max\, v_i - min\, v_i}$$

stardardization (mean 0, sd 1):

$$z(v_i) = \frac{x - \mu}{\sigma}$$

## Non numerical attributes

The distance between two nominal values is 1 if they are different and 0 if they are the same

# Decision Trees

Try to learn a decision tree from data

Basic iterative process:

- Select an attribute
- Create a branch for each value of the attribute
- Each branch includes a set of samples
- Repeat the process on each branch, taking only into account those samples under such branch
- If the samples are of the same class, stop

# Decision Trees

## Which attribute is the best?

We look for the attribute which gives more information about the class

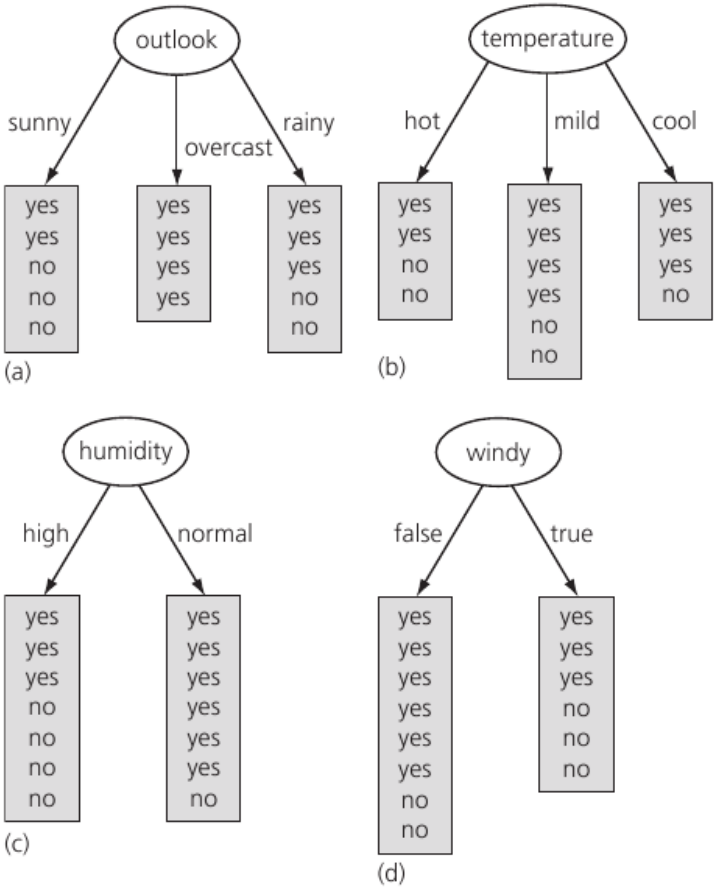
Information gain

We try that on each branch there is a dominant class

It is important to take into account all branches

Some branch can include samples of the same class but other branches don't

Branch-size weighted mean




*outlook* info 3 branches
info([2,3]) = 0.971 *sunny* branch
info([4,0]) = 0.0 *overcast* branch
info([3,2]) = 0.971 *rainy* branch
info(*outlook*) = info ([2,3], [4,0], [3,2]) = 5/14 * 0.971 + 4/14 * 0 5/14 *0.971 = 0.693

Root attribute: info(*root*) = info([9,5]) = 0.940
**Gain(*outlook*) = info(*root*) – info(*outlook*) = 0.940 – 0.693 = 0.247 //best option**
*Gain*(*temperature*) = 0.029 *Gain*(*humidity*) = 0.152 Gain(*windy*) = 0.048

# Decision Trees

## Function info([#classA, #classB, ..., #classN])

It should be:

- Multiclass
- If all are of the same class, it should return 0
- If all are distributed uniformly, it should be maximum
- It should meet the *step-by-step* evaluation property
  - Example (3 classes: A,B,C):
    - info([2,3,4]) = info([2,7]) + (7/9) * info([3,4])
    - First we decide A *vs.* "others" and then (in 7 of 9 cases) we decide if it is B or C
- An example of "info" function that meets these properties is *entropy*
  - entropy($[p_1,...,p_n]$) = $-p_1\log p_1$ - ... - $p_n\log p_n$
  - info($[p_1,...,p_n]$) = entropy($[p_1/N, ... , p_n/N]$), where $N = p_1+...+p_n$

# Decision Trees

If we have attributes with many possible values, we should make a correction

- Many branches promotes gain, which is an undesired effect
- We compute *gain ratio*.
  - gain_ratio(attribute) = gain(attribute) / split_info(attribute)
  - where:
    - split_info(attribute) = info([#branch1, ... , #branchN])
      - Necessary info to know which branch will be taken. It only takes into account how much members belong to each branch. The more branches, the more split_info, so less gain

| Outlook | | Temperature | | Humidity | | Windy | |
|---|---|---|---|---|---|---|---|
| info: | 0.693 | info: | 0.911 | info: | 0.788 | info: | 0.892 |
| gain: 0.940–0.693 | 0.247 | gain: 0.940–0.911 | 0.029 | gain: 0.940–0.788 | 0.152 | gain: 0.940–0.892 | 0.048 |
| split info: info([5,4,5]) | 1.577 | split info: info([4,6,4]) | 1.557 | split info: info ([7,7]) | 1.000 | split info: info([8,6]) | 0.985 |
| gain ratio: 0.247/1.577 | 0.157 | gain ratio: 0.029/1.557 | 0.019 | gain ratio: 0.152/1 | 0.152 | gain ratio: 0.048/0.985 | 0.049 |

# Linear

Work with numerical attributes

They are intended to classify samples that are *linearly separable*

Linear regression

The predicted value for a sample $i = (a_1, ..., a_k)$ will be:

$$predict\left(a^{(i)}\right) = w_0 + \sum_{j=1}^{k} w_j \cdot a_j^{(i)}$$

$w$ is a weight vector, which is computed by trying to minimize the training error ($x^{(i)}$ = class of sample $i$)

$$error = \sum_{i=1}^{n} \left(x^{(i)} - \left(w_0 + \sum_{j=1}^{k} w_j \cdot a_j^{(i)}\right)\right)$$

# Linear

## Linear Regression

### How to compute *w*?

### Gradient descent algorithm

Iterative algorithm to find the minimum of a function (the error function)
Briefly:

At each step, the error is computed and weights are updated in order to reduce this error.

The algorithm stops when the error is small enough or a maximum number of iterations is reached.

### How it works? It is based on the derivative of the *cost function*

The cost function is similar to the error given the weights, but we want it to be positive (independent of the direction of the error) and easily derivable

$$J(w, w_0) = \frac{1}{2} \sum_{i=1}^{n} \left( x^{(i)} - \left( w_0 + \sum_{j=1}^{k} w_j \cdot a_j^{(i)} \right) \right)^2$$

# Linear

## Linear Regression

### Gradient descent algorithm (cont)

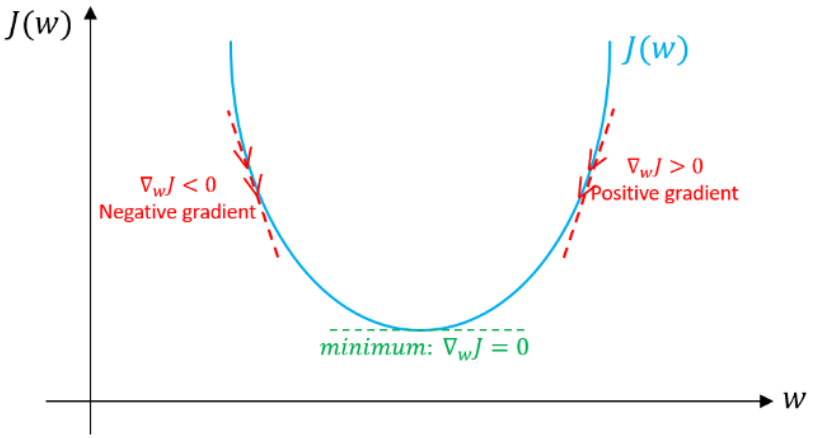
This algorithm needs the *gradient,* based on the *derivative* of the *cost function*

$$\frac{\partial J(w, w_0)}{\partial w_f} = -\sum_{i=1}^{n} \left( x^{(i)} - \left( w_0 + \sum_{j=1}^{k} w_j \cdot a_j^{(i)} \right) \right) a_f^{(i)}$$

Intuition: the derivative means how the cost varies when changing the weight $w_f$. It depends both on the amount of current error and how big are the values of the attribute in the training set.

At each iteration, each weight $w_f$ is updated in the *opposite direction of its partial derivative and at a learning rate* $\alpha$

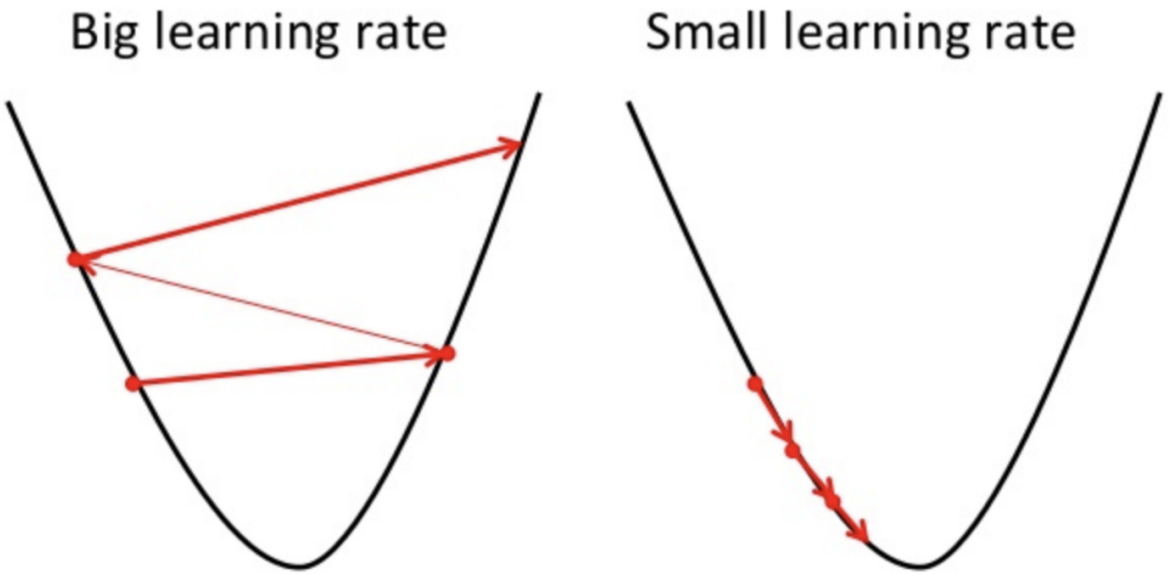
$$w_f := w_f - \alpha \frac{\partial J(w, w_0)}{\partial w_f}$$



# Linear

## Gradient descent algorithm (cont)

- The learning rate $\alpha$ must be carefully selected
  - Very small learning rates makes the training process slower
  - Very large learning rates makes the descent to jump over the minimum



# Linear

## Linear Regression

Adapting linear regression for classification seems to be easy: each data point is associated with 0 or 1, for each of the two possible classes

Problems:

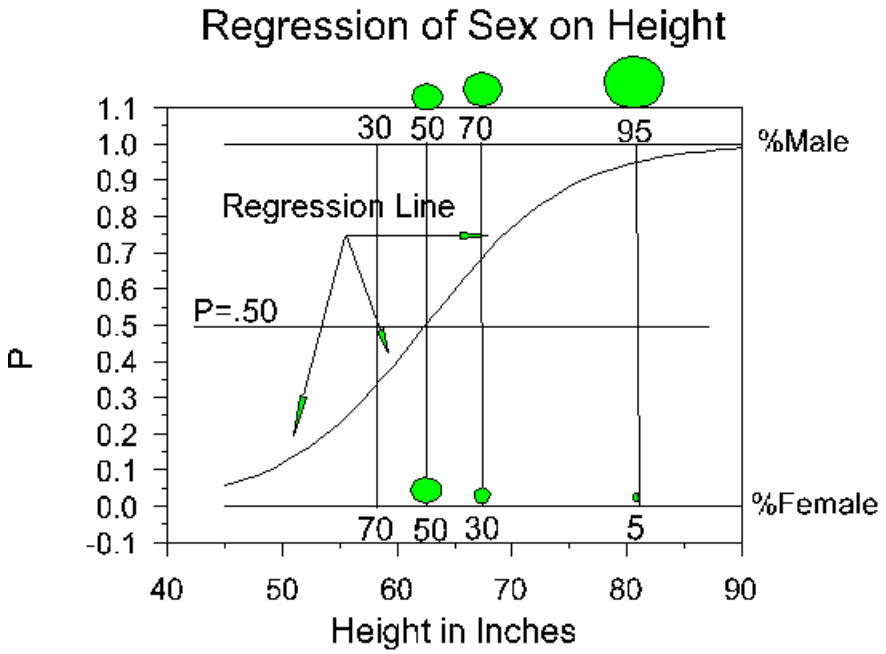
Linear regression does not gives values between 0 and 1, which are intuitively associated to a probability of belonging to a class.

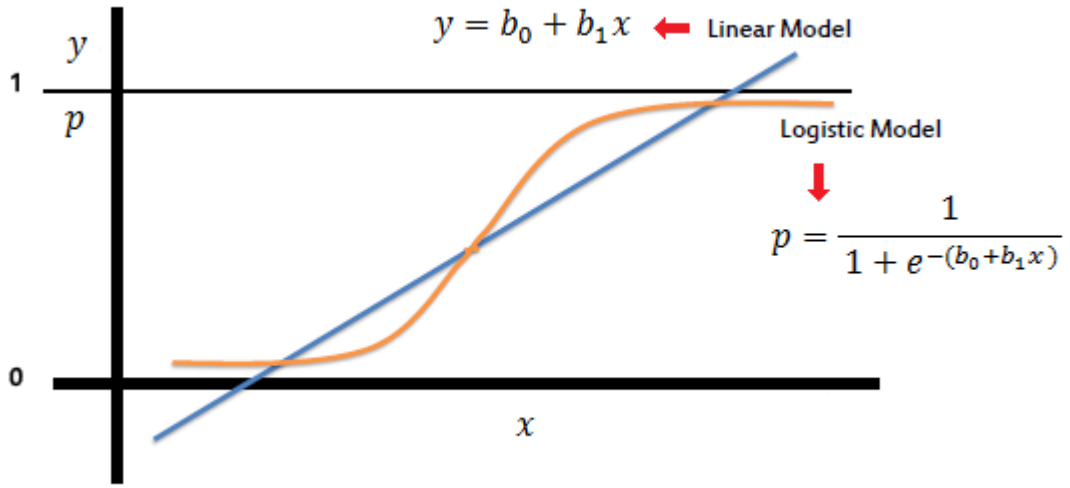
Not statistically sound: it assumes that error follows a normal distribution and the variance is constant, which is not true for binary outputs.

# Linear

## Logistic regression

### Graphical interpretation of the outcome



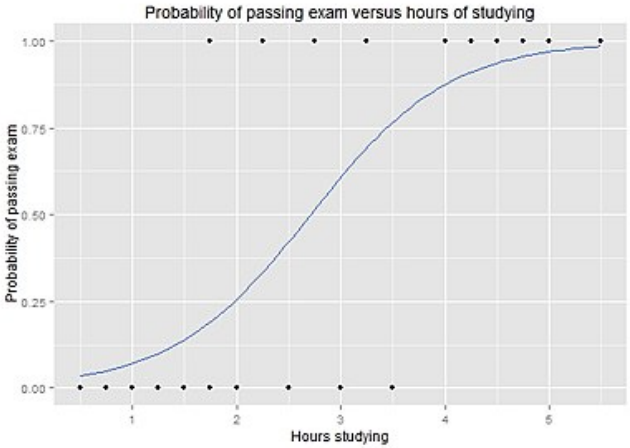

Linear regression vs. Logistic regression

# Linear

## Logistic regression

Gives output between 0 and 1. In bi-class, it can be assumed as the probability of belonging to class 1.

$$Pr(1|a^{(i)}) = \frac{1}{1+e^{-(w_0+w_1 \cdot a_1+\ldots+w_k \cdot a_k)}}$$




The cost function is different and based on logarithms, which gives high cost for confident wrong predictions:

$$J(w, w_0) = -\sum_{i=0}^{n} (1-x^{(i)}) \boxed{\log(1-Pr[1|a_1^{(i)}, a_2^{(i)}, \ldots, a_k^{(i)}])} + x^{(i)} \boxed{\log(Pr[1|a_1^{(i)}, a_2^{(i)}, \ldots, a_k^{(i)}])}$$

# Linear

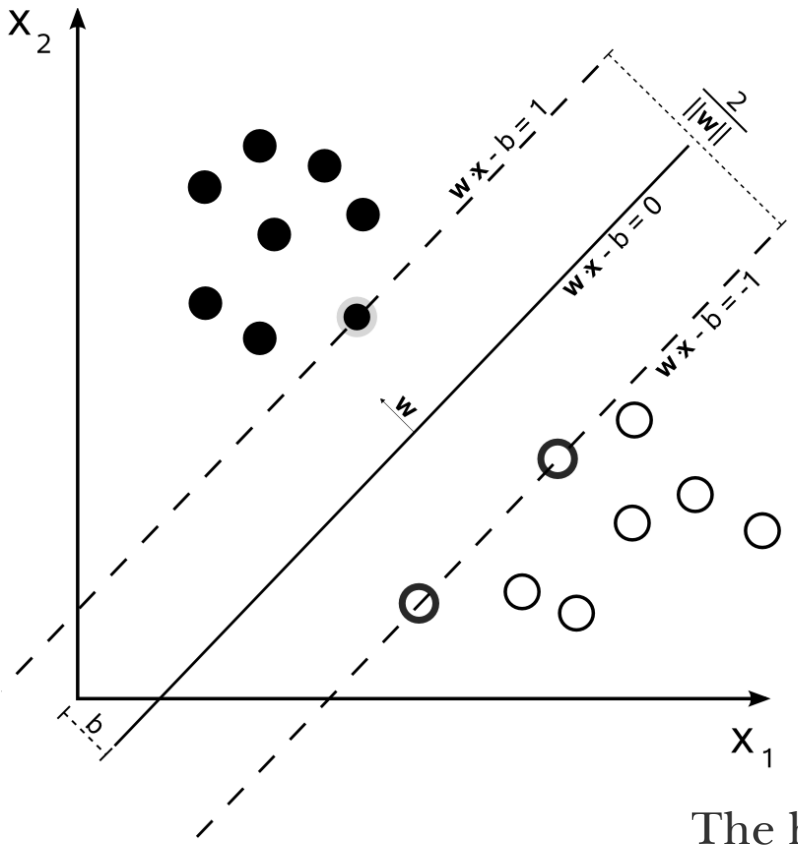
## Logistic regression

- For multiclass (K classes), there are several methods
  - Take a “pivot” class (say class K)
  - Do a regression for each other class (K-1 classes) against the pivot class (class K)
  - Adjust probabilities to sum up 1
  - Choose the class with major probability

# Linear

## Support Vector Machines (SVM)

### Binary classifier (easily extensible to multiclass)




Samples are represented in n-dimensional space (n = no. features)

Learn:

$$y = f(x),\ y \in \{\pm 1\},\ x \in \mathbb{R}^n$$

The objective is to find an hyperplane (n-1 dimension) which separates positive from negative instances.

Mathematically

Large margin

Find $(w, b)$, minimising: $\|w\|$

subject to: $y_i(w \cdot x_i - b) \geq 1$

The hyperplane separates each class instances

# Linear

## Support Vector Machines (SVM)

Once $w$ y $b$ are found, classification is given by:

$$f(x) = w \cdot x + b$$

Giving the value +1 if $f(x) > 0$, or -1 otherwise

# Linear

## Support Vector Machines (SVM)

If not all samples can be separated.

*Soft-margin* SVM. Allows an error that should be minimized. C parameter indicates the cost of an error during training.

Now the objective is:

$$\text{Find } (w, b), \text{ minimizing: } \|w\| + C \cdot \sum_{i=1}^{m} \xi_i$$

$$\text{subject to: } y_i (w \cdot x_i - b) \geq 1 - \xi_i, \xi_i \geq 0$$

# Linear

## Support Vector Machines (SVM)

### Non linear case

Alternative: Map input data to a higher dimensional space and try to find an hyperplane in that space

preprocess data:

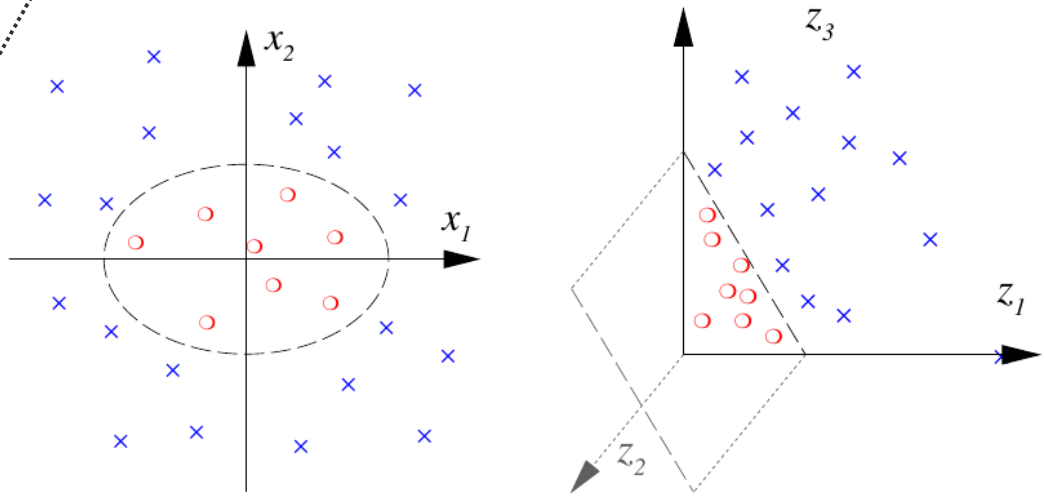
$$x \mapsto \Phi(x)$$

Find $w$
and the prediction function is:

$$f(x) = w \cdot \Phi(x) + b$$

Example: polynomial map

$$\Phi : R^2 \to R^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{(2)} x_1 x_2, x_2^2)$$



# Linear

## Support Vector Machines (SVM)

Problem: The map function could lead to a very high dimensionality, making it difficult to keep $w$ in memory and solve the optimization problem.

Solution: dual form + kernel trick

# Linear

## Support Vector Machines (SVM)

### Dual form. The optimization problem can be presented in its dual form, with Lagrangian multipliers

We try to find:

Find $\alpha_i$, minimising: $\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j x_i x_j$

subject to:

$$\sum_{i=1}^{m} y_i \alpha_i = 0$$

$$0 \le \alpha_i \le C, i = 1, \ldots, m$$

The classification function is now:

$$f(x) = \sum_{i}^{n} \alpha_i y_i x_i \cdot x + b$$

Moreover, there is a relation between $w$ y $\alpha$

$$w = \sum_{i=1}^{n} \alpha_i y_i x_i$$

# Linear

## Support Vector Machines (SVM)

### Dual form

Advantage: Both in the function to solve and the decision function data appear as dot products

$$\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j x_i \cdot x_j$$

$$f(x) = \sum_i \alpha_i y_i x_i \cdot x + b$$

For the non linear problem, we include a map $\boldsymbol{\Phi}$:

$$\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \Phi(x_i) \cdot \Phi(x_j)$$

$$f(x) = \sum_i \alpha_i y_i \Phi(x_i) \cdot \Phi(x) + b$$

# Linear

## Support Vector Machines (SVM)

### Kernel trick

Lets consider the function K (kernel):

$$K(x_i, x) = \Phi(x_i) \cdot \Phi(x)$$

If K is the dot product, we maintain the problem in the same input space, but by varying K we could get something like:

Map + dot product (but without making an explicit mapping!)

Example:

Polynomial kernel:

$$K(x, x') = (x \cdot x')^2$$

Which is equivalent to the previous mapping:

$$\Phi : \mathbb{R}^2 \to \mathbb{R}^3 \quad (x_1, x_2) \to (z_1, z_2, z_3) := (x_1^2, \sqrt{2}\, x_1 x_2, x_2^2)$$

# Linear

## Support Vector Machines (SVM)

### Kernel trick:

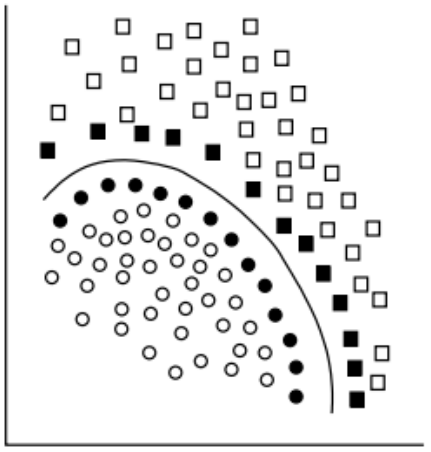
#### Other kernels.

Polynomial

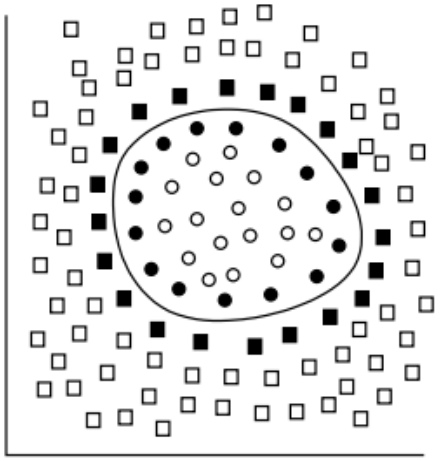
$$K(x, x') = (x \cdot x' + c)^q$$

RBF (adds a small "hill" on each point)

$$K(x, x') = e^{-\gamma \|x_i - x\|^2}$$



polinomial

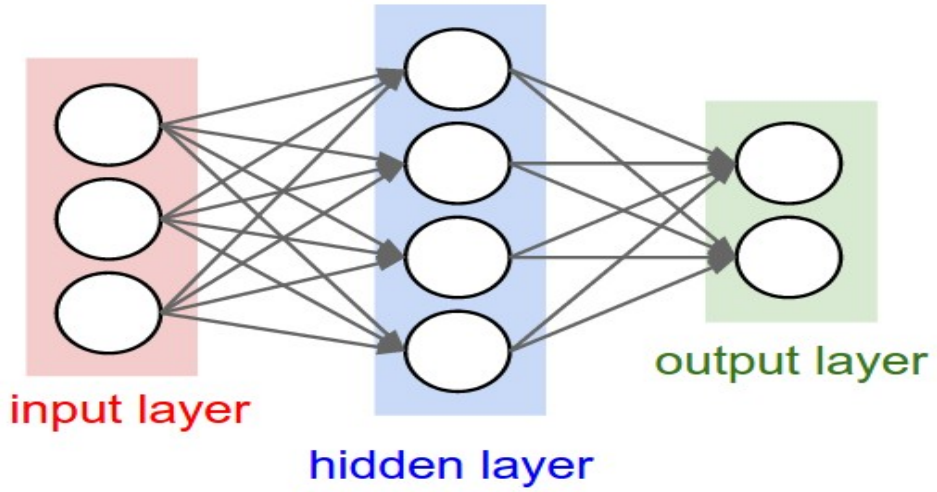


RBF

# Linear

## Neural Networks

- A neural network can be seen as a complex linear classifier able to learn non-linear, multi-class datasets
- It also uses gradient descent for training
- Basic architecture
  - Neurons disposed in layers
  - The input layer receives a sample
    - For example: each gene expression value
  - The hidden layer(s) combine(s) the output from previous layers
  - The output layer gives predictions
    - For example: one output neuron gives the score for each possible class (patient possible conditions)



# Linear

## Neural Networks

Each neuron is composed with a set of weights $w$, a bias $b$ and an **activation function** $f$ (a.ka. Non-linearity)

Neuron output (known as "activation"):

$$a(x)=f\left(\sum_i w_i x_i+b\right)$$

Possible activation functions $f$:

Sigmoid

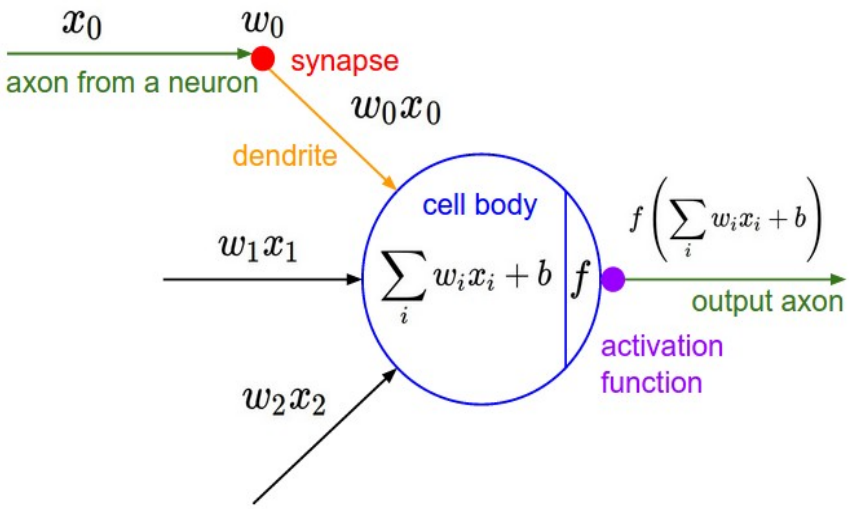
$$\sigma(x)=\frac{1}{(1+e^{-x})}$$

Tanh

$$\tanh(x)=2\,\sigma(2x)-1$$

ReLU (Rectified Linear Unit)

$$f(x)=max(0,x)$$



# Linear

## Neural Networks

### Training. Backpropagation algorithm

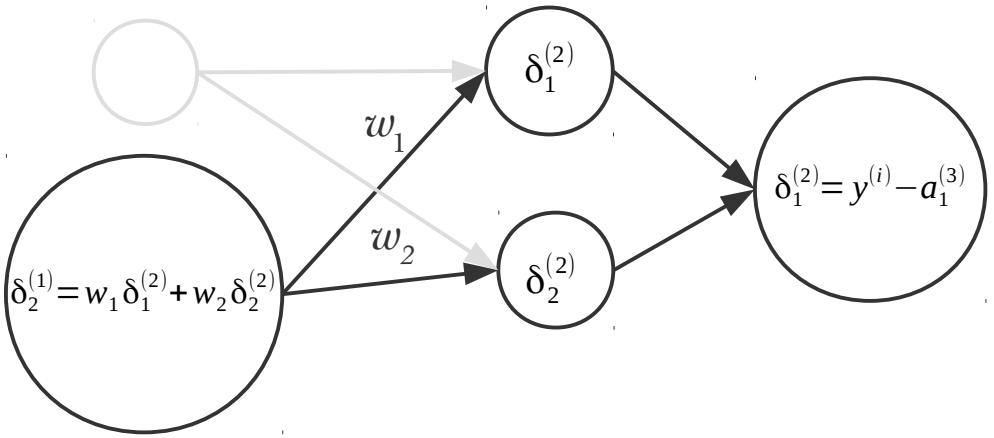
It is a method to compute the partial derivative (δ) at each neuron in order to update its weights with gradient descent (as in previous methods)

δ is calculated from the last layer down to the first

In the last layer, the gradient depends only on the expected output

In intermediate layers, the gradient depends on the gradient of the next connected neurons, weighted by the connection's weights

Intuition:



# Linear

## Neural Networks

### Training. Backpropagation algorithm

Once $\delta_n$ is calculated for each neuron $n$, and given that (which is proven):

$$\frac{\partial J}{\partial w_{ij}^{(L)}} = \delta_n^{(L)} a_n$$

We can apply gradient descent to update weights a learning rate $\alpha$

$$w_{ij} := w_{ij} - \alpha \delta_n^{(L)} a_n$$

# Linear

## Convolutional Neural Networks (CNN)

*Deep Learning*: subfield of Machine Learning able to learn from datasets without doing *feature engineering*

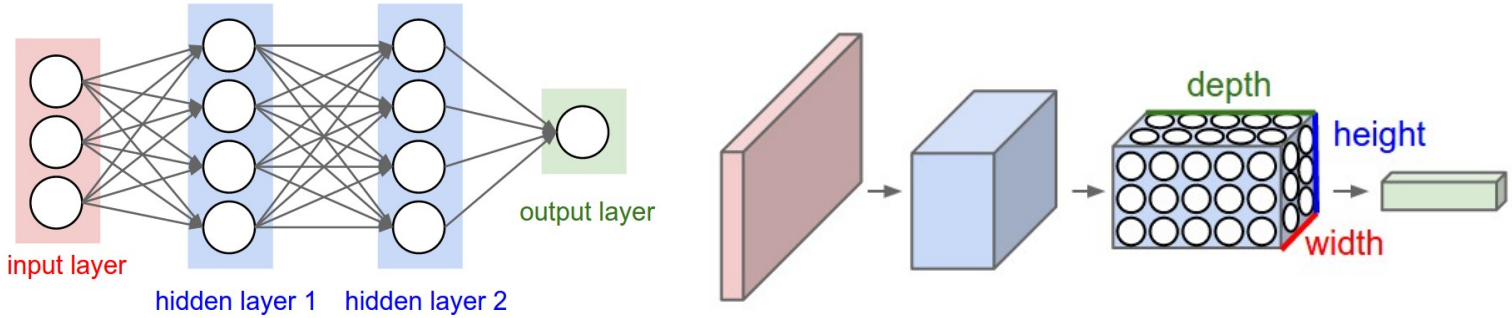
For example, in order to detect objects in an image, a preprocessing step trying to find basic shapes (features) focusing on the specific task was explicitly programmed. Deep Learning techniques try to avoid this step, working with raw data directly.

Convolutional Neural Network (CNN): A special type of *deep* neural network intended for image processing.

# Linear

CNN vs classic Neural Networks. Key differences:

- In CNN, layers are *volumes* of neurons having width, height and depth.
- Neurons are not *fully connected* to the previous layer, because it will not scale well for images (huge number of connections).
  - They only process a square portion of the input.
- Weights are *shared*. Neurons at the same depth in the same volume *share* they weights.
  - It is reasonable for image processing as well as it reduces dramatically the number of parameters.



# Linear

## Convolutional Neural Networks (CNN)

### Types of layers in a CNN:

#### Convolutional Layer.

The most important layer. Neurons are connected to portions of the input volume.

#### RELU layer.

Applies an elementwise activation, such as max(0, x). The input volume's dimensions are not changed

#### POOL layer.

Reduces the the spatial dimensions (width and height).

#### Fully connected layer.

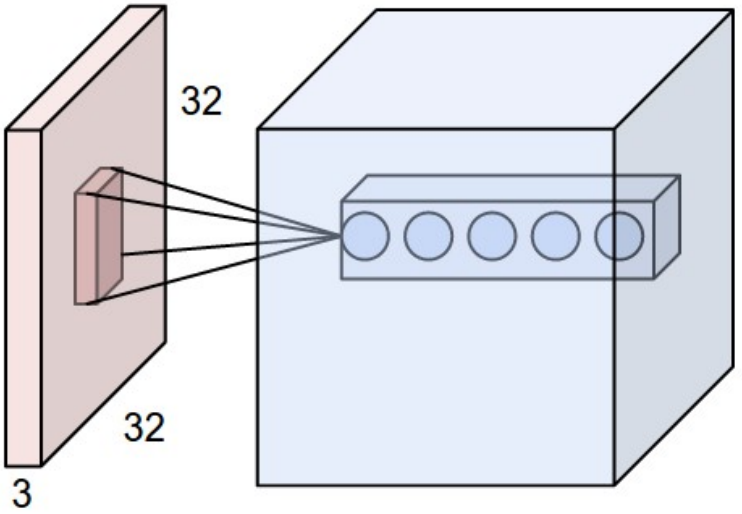
Typical final layer, which is fully connected to the input and has a neuron per desired output (for example, 10 neurons for a 10-class classification problem)

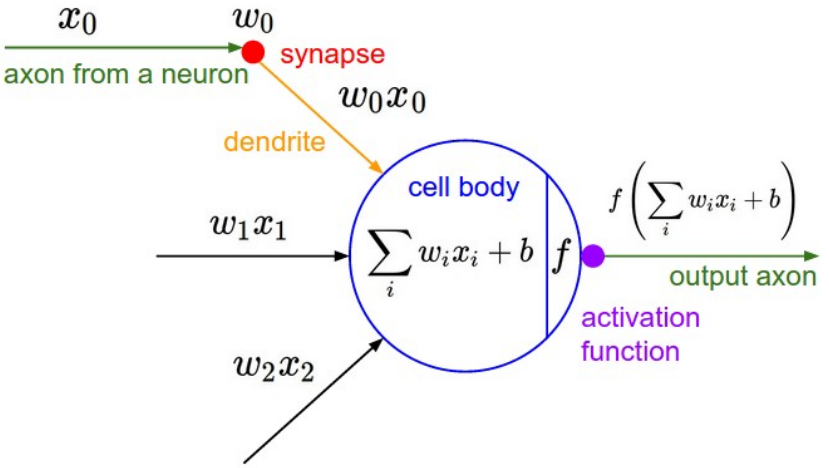
# Linear

## Convolutional Neural Networks (CNN)

### Convolutional Layer

- Each neuron receives a small portion of the input's width and height (but all the input's depth)
- Neurons in at the same depth in the conv. layer share they weights.
- Each set of neurons at the same depth is called *a filter*
  - They process the input image applying the same operation in a sliding window (convolution), so they are like applying a filter to the image

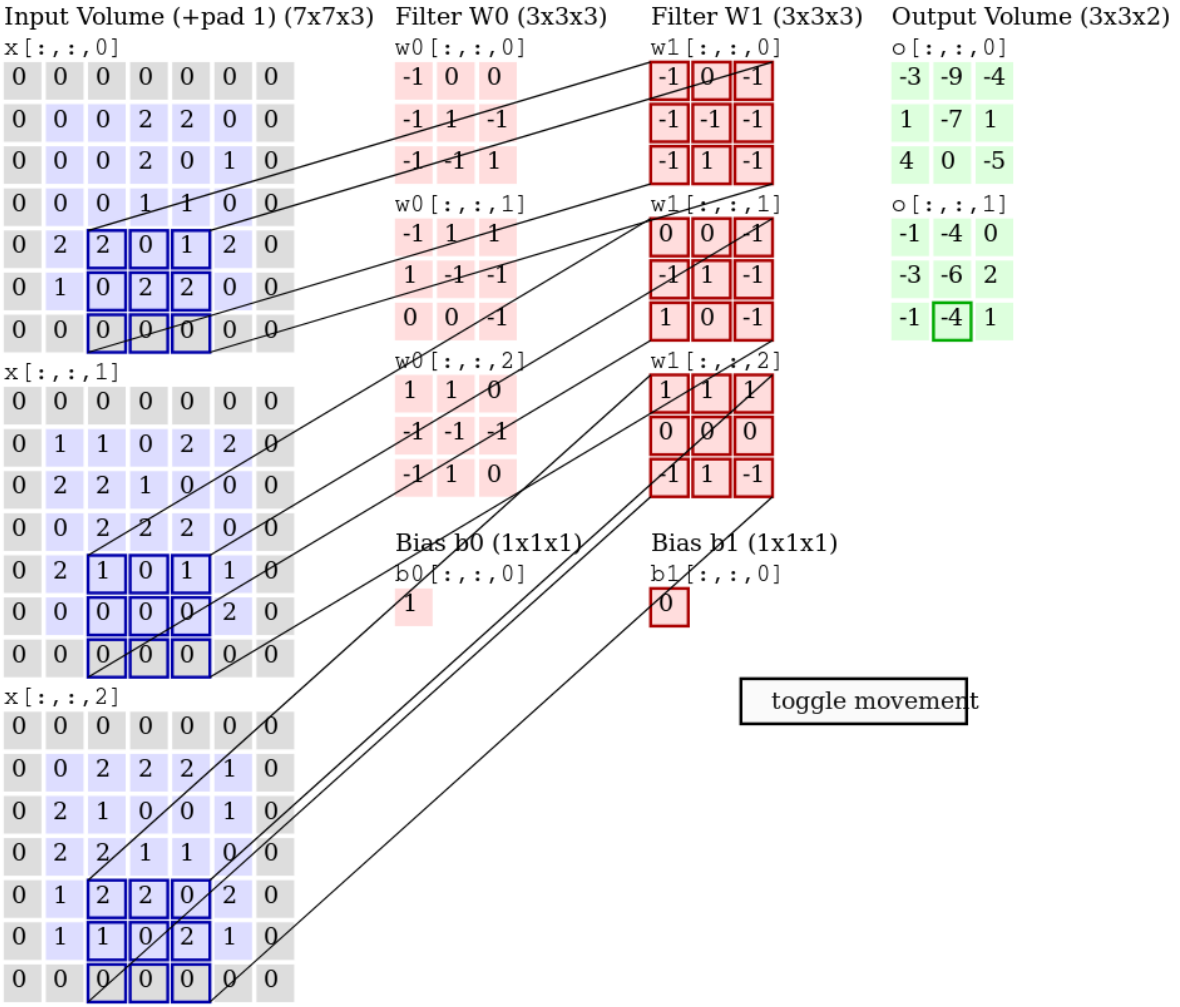


# Linear

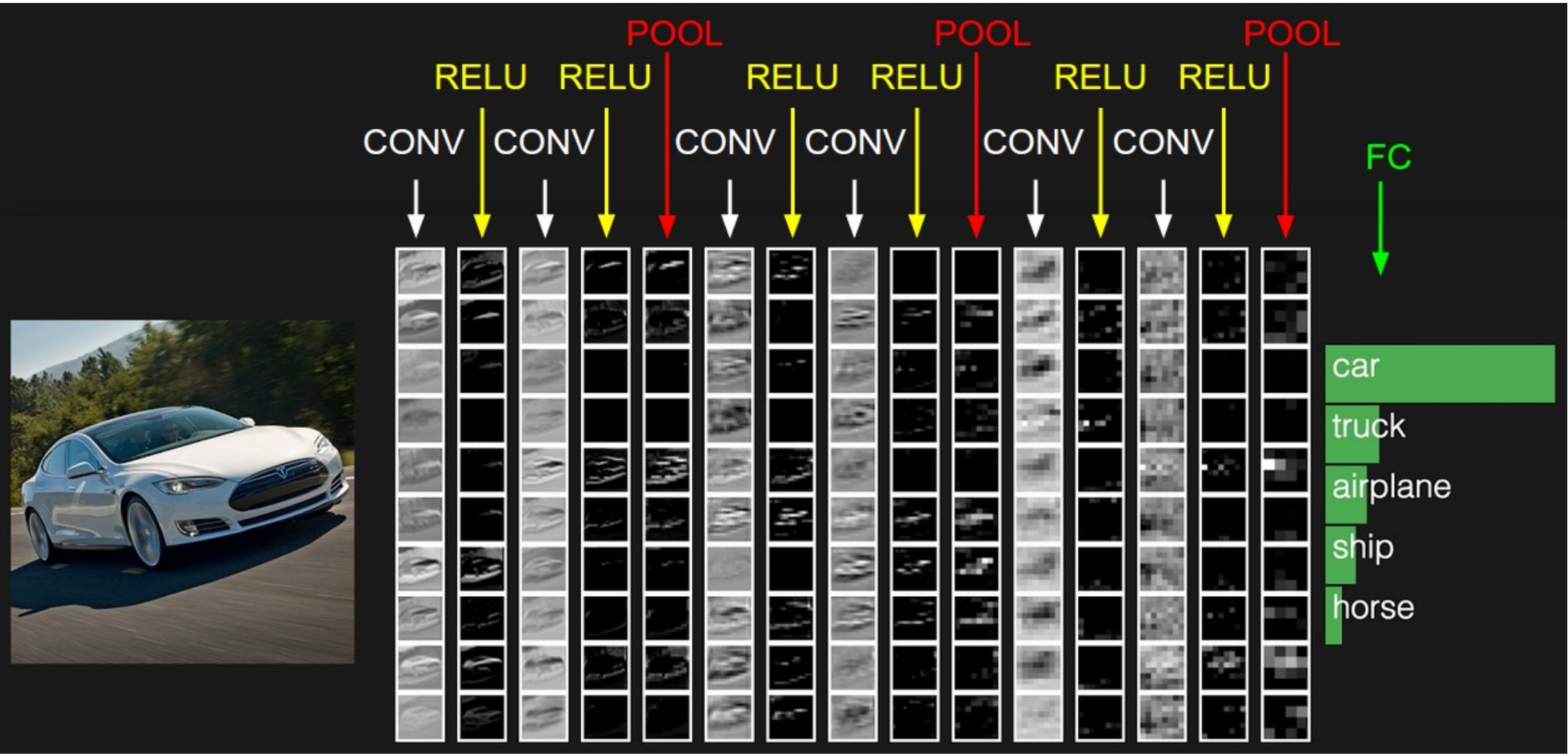
## Convolutional Neural Networks (CNN)

### Example of convolutional layer values



# Linear

## Convolutional Neural Networks (CNN)



# Classifier ensembles

## Employ several classifiers in order to improve performance

**Ensemble** vs. other classifier combination approaches:

Ensembles employ many classifiers (of one or several types). Moreover, its number usually varies depending on the training data

The combination of a reduced number of classifiers is not considered an ensemble (less than 10), specially when they are intended to integrate data from heterogeneous sources

## Motivation:

### Improve the statistical performance

Probably, the performance of the classifier combination is lower than a specific classifier, but the risk of choosing a bad classifier is reduced

### Computational aspects

Usually it is unfeasible to try all classifiers to see which is the best one. By combining several types, the risk is reduced

### Representation capabilities: divide and conquer

Making each classifier to focus on a subpart of the input data space, **results can be improved**

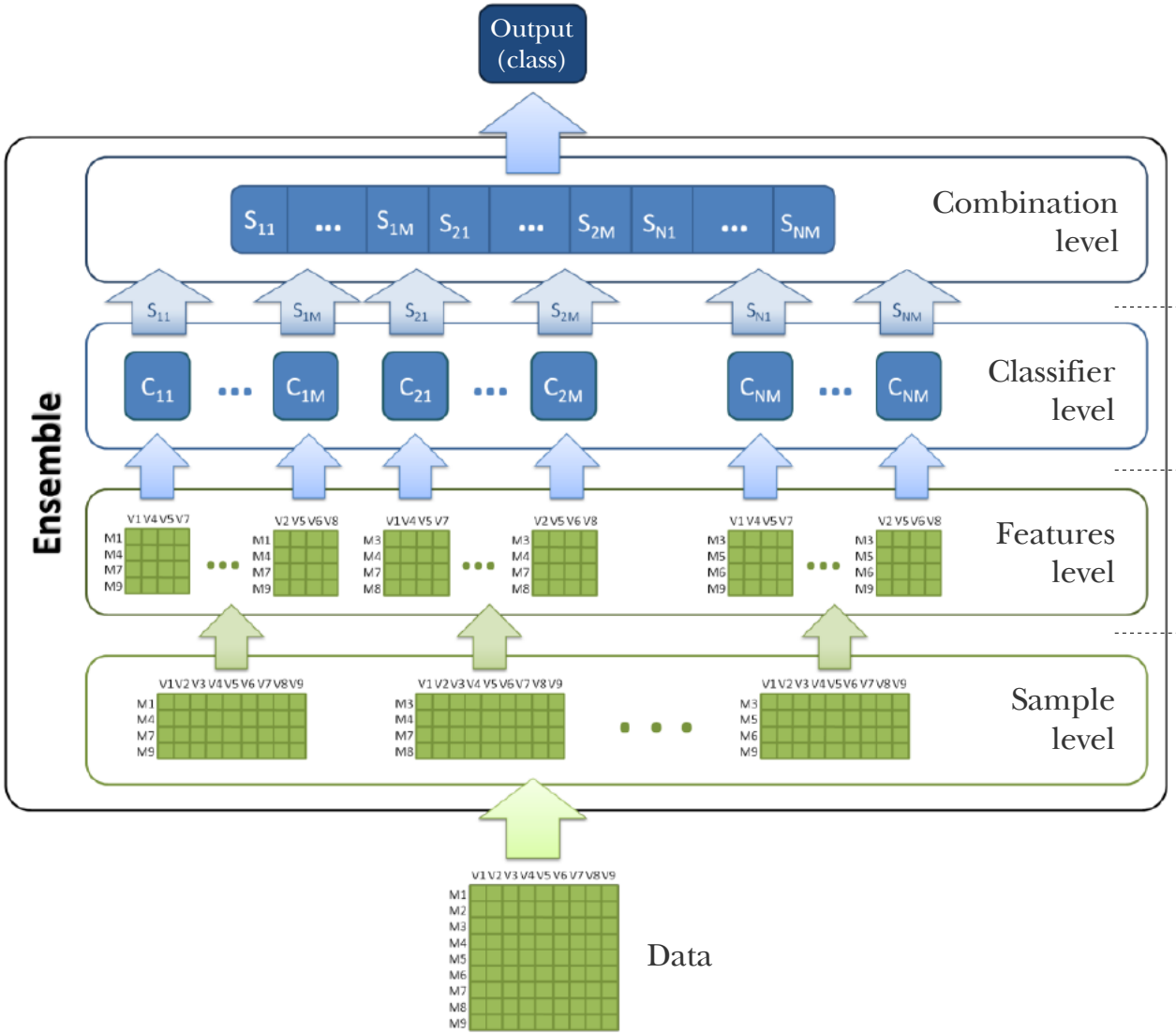
### Advantages regarding data volume

Very high data volume. Scalability, due to the possibility of train several classifiers per data subspace concurrently

Very low data volume. Resampling data and train a classifier on each sample

# Classifier ensembles

## Ensembles general framework




Output type:
(I) class, (II) ranking p.class, (III) p. class confidence.
Distinct methods for each type

Homogeneous vs. Heterogeneous
Construction: Independent vs. Dependent
Classification: Parallel vs. Sequential vs. div. and conq.

Natural grouping (problem dependent)
Random selection
Not random (favourite class, iterative, incremental)
By optimization (opt. diversity and performance)

Sampling methods (with replacement)
Weights usage
Partition methods (without replacement)
New sample creation methods

# Classifier ensembles

## Diversity

Central and desired feature in classifier ensembles

If we find a set of classifiers diverse enough, that do not make the same errors, then we can improve the performance of the base classifiers

How to achieve diversity:

- Modify classifier parameters
- Modify input training data (sampling, partition, creation).
- Divide search space (divide and conquer)
- Mix several types of classifiers

# Classifier ensembles

## Diversity

### Measuring diversity

#### For each pair of classifiers:

Taking this matrix:

| | $C_j$ hit (1) | $C_j$ fail (0) |
|---|---|---|
| $C_i$ hit (1) | $N^{11}$ | $N^{10}$ |
| $C_i$ fail (0) | $N^{01}$ | $N^{00}$ |

$$Q_{i,j} = \frac{N^{11}N^{00} - N^{01}N^{10}}{N^{11}N^{00} + N^{01}N^{10}}$$

Q statistic [-1, 1].
0 = independent

$$\rho_{i,j} = \frac{N^{11}N^{00} - N^{01}N^{10}}{\sqrt{(N^{11}+N^{10})(N^{01}+N^{00})(N^{11}+N^{01})(N^{10}+N^{00})}}$$

ρ correlation coefficient
Similar to Q

$$Des_{i,j} = \frac{N^{01}+N^{10}}{N}$$

Disagreement score

$$DF_{i,j} = \frac{N^{00}}{N}$$

Doble fault

#### Joint diversity of two classifiers

$$E = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{C - \lceil C/2 \rceil}\min\{F_i, (C - F_i)\}$$

Entropy

$$KW = \frac{1}{NT^2}\sum_{i=1}^{N} F_i \cdot (C - F_i)$$

Kohavi-Wolpert Variance (T=number of classifiers)

($F_i$ number of classifiers failing $i$ sample).

# Classifier ensembles

## Some examples

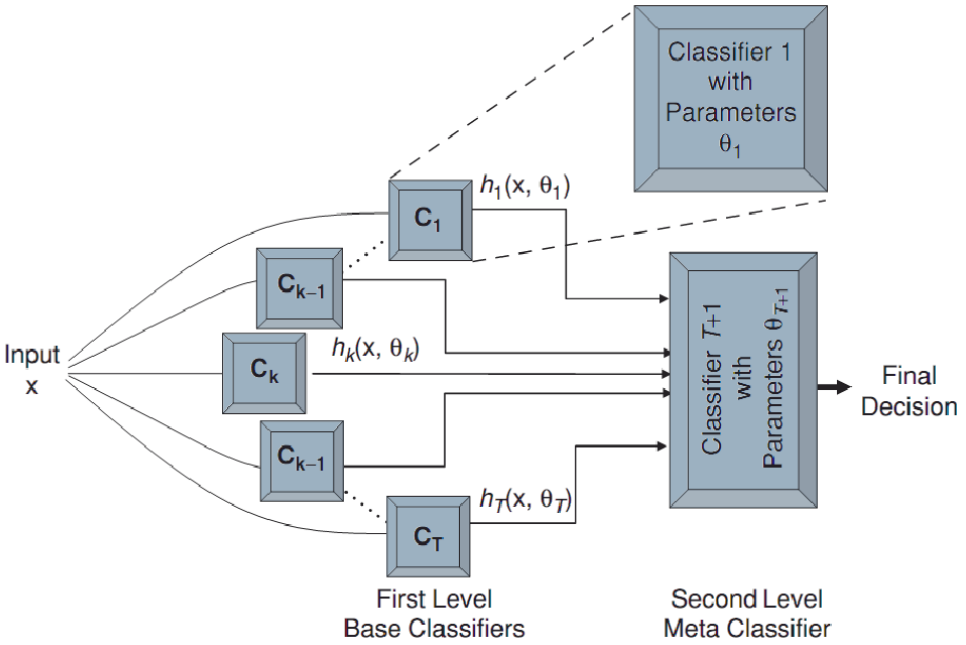
- Bagging (Bootstrap AGGregatING)
  - Several classifiers over subsamples by using resampling with replacement
  - Combining by majority vote
- Random Forest
  - Bagging variation
  - Builds multiple decision trees by varying:
    - Parameters randomly
    - Taking a subset of samples and/or attributes randomly
- AdaBoost
  - Sequential training of several classifiers of the same type and parameters
  - On each iteration failing samples of the previous iteration have more weight
  - Combination by performance-weighted voting

# Classifier ensembles

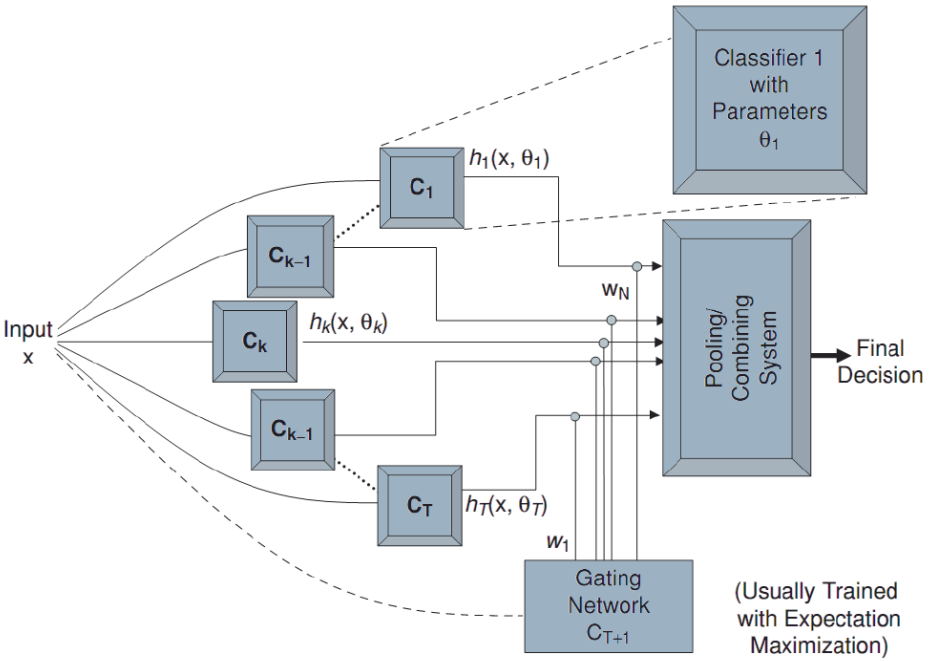
## Some examples

### Non-ensemble approaches

**Stacking**
A classifier learns how to generate a classification taking as input the output of base classifiers




**Mixture of experts**
A neural network learns which classifiers should vote given input data



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# Machine Learning

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