# Introduction to Artificial Intelligence (ENSIMAG)
# Intelligent Systems (MOSIG)

Some models for unsupervised and supervised learning

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Lecture: Pierre Gaillard

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## Outline

## Supervised and unsupervised learning

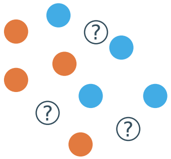
Make sense of the data

## Supervised vs unsupervised learning

**Two main categories** of machine learning algorithms:

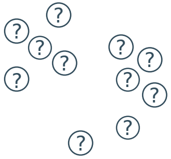
- **Supervised learning:** predict output $Y$ from some input data $X$. The training data has a known label $Y$.

  Examples:
  - $X$ is a picture, and $Y$ is a cat or a dog
  - $X$ is a picture, and $Y \in \{0, \dots, 9\}$ is a digit
  - $X$ is are videos captured by a robot playing table tennis, and $Y$ are the parameters of the robots to return the ball correctly



- **Unsupervised learning:** training data is not labeled and does not have a known result

  Examples:
  - detect change points in a non-stationary time-series
  - detect outliers
  - clustering: group data in homogeneous groups
  - principal component analysis: compress data without loosing much information
  - density estimation
  - dictionary learning



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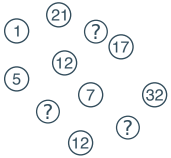

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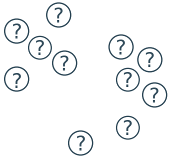

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## Supervised vs unsupervised learning

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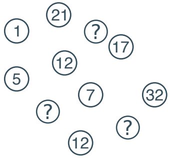
- **Supervised learning:** predict output $Y$ from some input data $X$. The training data has a known label $Y$.

| Classification | Regression |
|---|---|
| KNN, SVM, Neural Nets, Logistic regression, Decision Trees, Random Forest, ... | Lasso, Ridge<br>Nearest Neighbors<br>Neural Networks,... |



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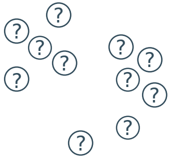
| Clustering | Dimensionality reduction |
|---|---|
| K-means, the Apriori algorithm, Birch, Ward, Spectral Cluster | PCA, IC, word embedding... |



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## Supervised learning

## Goal

Mostly, the same as the unsupervised case:

The goal as usual, is to make sense of the data.

For this we define a model

$$\mathcal{M}(\theta)$$

that have some parameter $\theta$, and we try to get the model fit to the data by **minimizing a loss**.

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Which model? Which loss?

## Classification

Let:

- $X$ be an $D$-dimensional random variable,
- and $Y$ binary (0/1) random variable.

$X$ and $Y$ are linked by some unknown *joint* distribution.

A predictor can be thought as a parametrized model $\mathcal{M}(\theta)$ of the conditional distribution $Y|X$.
The loss is usually chosen as the negative log-likelihood of the data:

$$-\sum_i \log p_\theta(Y = y_i | X = x_i)$$

$$\mathcal{M}(\theta) = P(Y = 1|X, \theta)$$

$$P(Y = 1|X, \theta) + P(Y = 0|X, \theta) = 1$$

## Logistic regression – Example

| Hours ($x_i$) | 0.50 | 0.75 | 1.25 | 1.75 | 2.00 | 2.5 | 3.75 | 4.00 | 5.00 | 5.50 |
|---|---|---|---|---|---|---|---|---|---|---|
| Pass ($y_i$) | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 1 | 1 | 1 |

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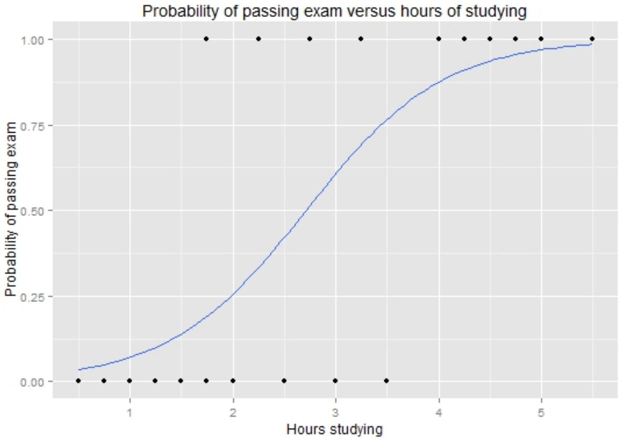
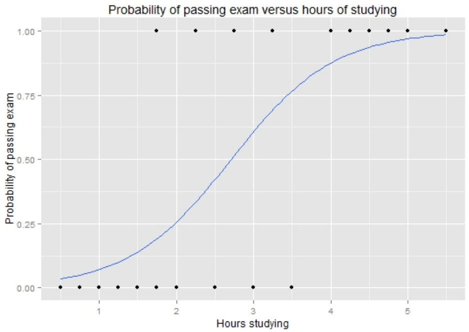


[Source: Wikipedia]

## Logistic regression – Example



The probability to pass the exam can be modeled by

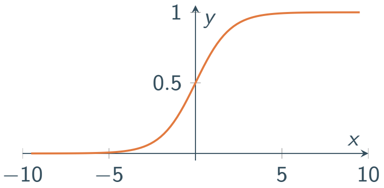
$$p(Y = 1|x) = \frac{1}{1 + e^{-(w \cdot x + b)}}$$

## Logistic regression

So we write

$$p(Y = 1|x) = \sigma(w \cdot x + b)$$

where the function $\sigma$ is the logistic sigmoid $\sigma : x \mapsto \frac{1}{1+e^{-x}}$



Sigmoid function

**Exercice**

Let $f$ be the predictor $f_{w,b}(x) = p(Y = 1|x) = \sigma(w \cdot x + b)$. Consider the case where $x \in \mathbb{R}^{\mathbb{D}}$ and interpret geometrically the role of parameters $w$ and $b$.

## Conditional likelihood

To measure the goodness of a fit we use the likelihood function, given by the probability that the set is produced by a logistic function:

$$\begin{aligned} L = P(y_1, ..., y_N | x_1, ... x_N, w, b) &= \prod_{i=1}^{N} P(y_i | x_i, w, b) \\ &= \prod_{i:y_i=1} p_i \prod_{i:y_i=0} (1 - p_i) \end{aligned}$$

We want to find $\theta = (w, b)$ such that $\mathcal{M}(\theta) = p$ maximizes $L$ for the observed data.

## Conditional likelihood

**Exercise**

1. Let $f(x) = p(Y = 1|x) = \sigma(w \cdot x + b)$. Show that the *conditional* log-likelihood $LL = \log P(y_1, ..., y_N | x_1, ..., x_N, w, b)$ can be written as:

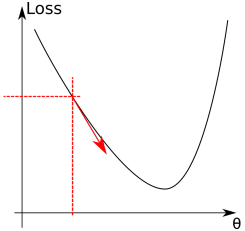
$$LL(w, b) = -\sum_{i=1}^{N} [y_i . \log f(x_i) + (1 - y_i) \log(1 - f(x_i))]$$

The name of the loss $\mathcal{L}(w, b; x) = -LL(w, b)$ is called the logistic loss, or binary cross-entropy.

2. Show that if $X|Y = i \sim \mathcal{N}(\mu_i, \Sigma)$, then $p(Y = 1|x)$ can be written as $\sigma(w \cdot x + b)$. Determine $w$ and $b$.
Hint: start by writing $p(Y = 1|x)$ using the Bayes rule.

## Logistic regression algorithmics

The conditional negative log likelihood of the logistic regression is convex, having a unique minimum.



Can be optimized with gradient descent (first order)

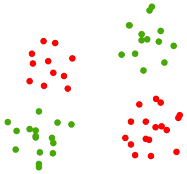
Even speed up by a Newton-Raphson scheme (second order as we can compute the Hessian) $\rightarrow$ leads to an algorithm [Rubin, 83] called *Iterative Reweighted Least Squares*.

## Issues with LR: linear separability

Other linear methods exist:

- Perceptron (lectures about neural networks)
- Fisher's Linear Discriminant

Most of the time, points are not linearly separable (thus, cannot be learnt with logistic regression):



## Toward kernel methods

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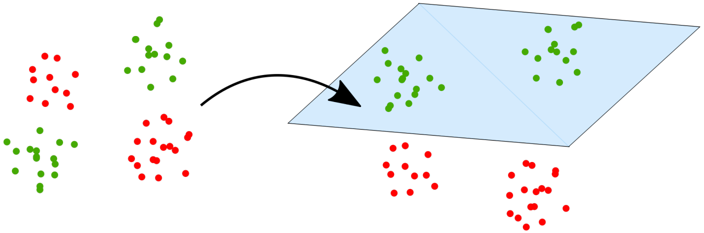

The idea is to replace the terms $x_i$ by a transformed version $\Phi(x_i)$ in a higher dimensional space (feature map chosen so that hopefully the data is more linearly separable), and learn a linear classifier there.

## Which feature map?

We don't design the feature map by hand.

Feature maps are usually chosen in families of feature maps known for:

- easing linear separation
- their computational tractability (see kernel trick just after)

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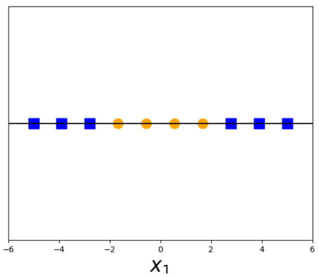
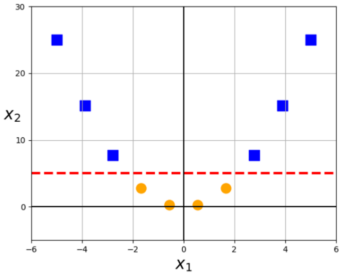
Indeed, $\Phi$ can project to a high (possibly infinity) dimensional space, that make the parameters and the scalar product $\langle w, \Phi(x_i)\rangle$ costly/impossible to compute.

## Which feature map?

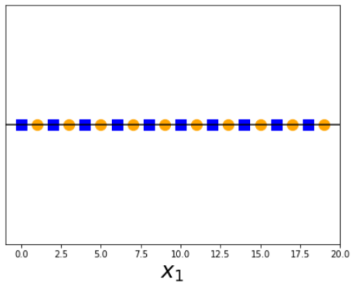


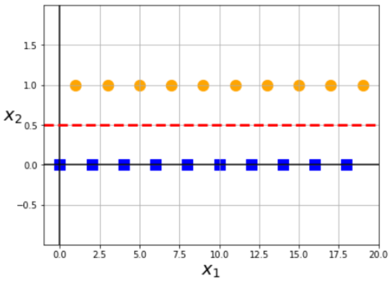


$$\Phi(x) = x^2$$

[Images from https://towardsdatascience.com/the-kernel-trick-c98cdbcaeb3f]

## Which feature map?

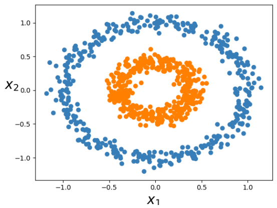


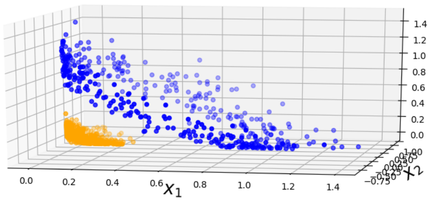


$$\Phi(x) = x \mod 2$$

[Images from https://towardsdatascience.com/the-kernel-trick-c98cdbcaeb3f]

## Which feature map?





$$\Phi(x) = \Phi((x_1, x_2)) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

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1.Reformulate the loss (dual formulation) so that it involves only a **linear combination of terms** of the form $\langle \Phi(x_i), \Phi(x_j) \rangle$ (no $w$, $b$ anymore, but $\Phi$ comes with it's own parameters).

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**Kernel trick**

Instead of choosing a feature map, and computing the scalar product, we choose a *kernel* that computes from 2 low dimensional vectors their scalar product in high dimension **without explicitly** computing the feature map.

Formally, we have data $\mathbf{x_i}, \mathbf{x_j} \in \mathbb{R}^D$ and a map $\Phi : \mathbb{R}^D \to \mathbb{R}^E$, then a **kernel function** is

$$k(\mathbf{x_i}, \mathbf{x_j}) = \langle \Phi(\mathbf{x_i}), \Phi(\mathbf{x_j}) \rangle$$

## Kernel example

Kernel trick for a 2nd degree polynomial mapping:

$$\begin{aligned} k(x_i, x_j) = \langle \Phi(a), \Phi(b) \rangle &= \begin{bmatrix} a_1^2, \\ \sqrt{2} a_1 a_2 \\ a_2^2 \end{bmatrix}^T \begin{bmatrix} b_1^2, \\ \sqrt{2} b_1 b_2 \\ b_2^2 \end{bmatrix} = \\ &= a_1^2 b_1^2 + 2 a_1 b_1 a_2 b_2 + a_2^2 b_2^2 = \\ &= (a_1 b_1 + a_2 b_2)^2 = \left( \begin{bmatrix} a_1, \\ a_2 \end{bmatrix}^T \begin{bmatrix} b_1, \\ b_2 \end{bmatrix} \right)^2 = \\ &= \langle a, b \rangle^2 = \langle x_i, x_j \rangle^2 \end{aligned}$$

Another common example is the Gaussian Kernel

$$k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle = \exp\left( -\gamma ||x_i - x_j||^2 \right)$$

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There are not established, general rules to know what kernel will work best for your particular data.

## Solving kernel methods

The solution of the dual problem (formulation omitted for this unit)

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

The decision boundary for a new point is

$$\mathbf{w}^T \mathbf{x} + w_0 = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x_i}^\mathbf{T} \mathbf{x} + w_0$$

The decision:

$$y = \text{sign}\left[\sum_{i=1}^{N} \alpha_i y_i \mathbf{x_i}^\mathbf{T} \mathbf{x} + w_0\right]$$

Mapping to feature space we have the decision

$$y = \text{sign}\left[\sum_{i=1}^{N} \alpha_i y_i \langle \Phi(\mathbf{x}), \Phi(\mathbf{x_i}) \rangle + w_0\right]$$

## Toward SVM (support vector models)

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- Supervised model for classification
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**New issue:**

Due to the kernel, the prediction of the class of a point $x$ cannot be written

$$\sigma(\langle w, \Phi(x)\rangle + b)$$

but it involves the computation of

$$\sum_{i=1}^{N} \alpha_i y_i k(x, x_i)$$

where $N$ is the size of the training set...

**SVMs to the rescue**

SVM solves this.

## SVM: Support vectors

To avoid the computation of $N$ terms when predicting: the loss is such that the model chooses few data points (called *support vectors*) that will play a role in the loss, the other are discarded.

**SVM**

SVM finds a linear separation between classes such that it maximizes the distance to the separation hyperplane (called the margin).

Instead of describing the hyperplane with a (potentially infinite) vector $w$, it writes it as a linear combination of support vectors (picked in the data).

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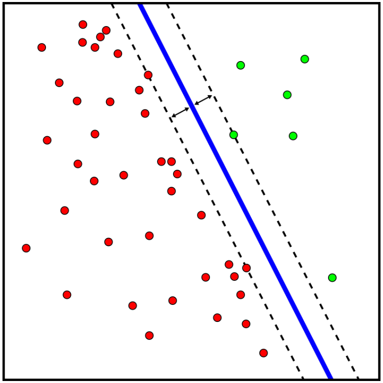
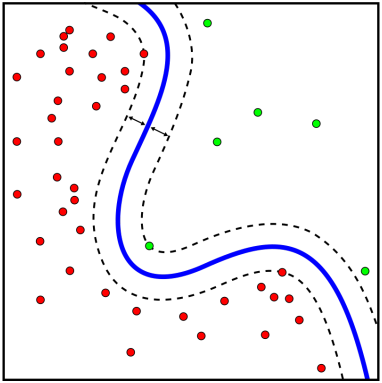
With a **Support Vector** set $\mathbf{SV} \subset \mathbf{X}$ we have

$$y = \text{sign}\left[\sum_{i \in \mathbf{SV}} \alpha_i y_i \langle \Phi(\mathbf{x}), \Phi(\mathbf{x_i}) \rangle + w_0\right]$$

## SVM visually


Identity feature map $\Phi(x) = x$ (linear kernel)

## SVM visually

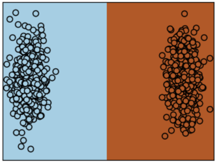


Gaussian kernel: $k(x_i, x_j) = e^{-\gamma||x_i - x_j||^2}$

The blue line is a plane in higher dimensional space, projected in 2D.

## Influence of noise

"Robust" separation



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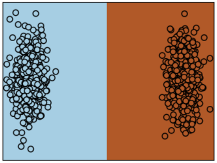
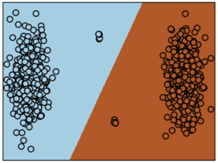


With few noisy points



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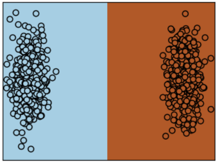

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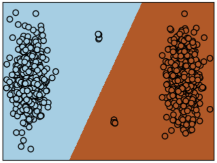
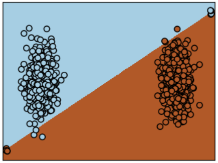
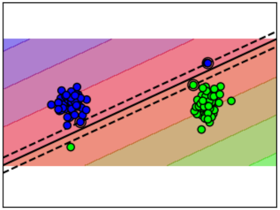


Even more



## Soft margins

To solve the issue of robustness to points near the decision boundary, one can introduce an hyper-parameter that controls the tolerance to misclassification (during inference). Without entering into details, visually it amounts to:



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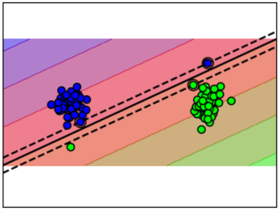

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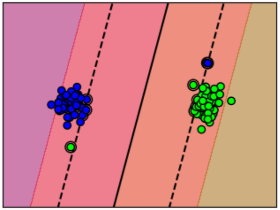
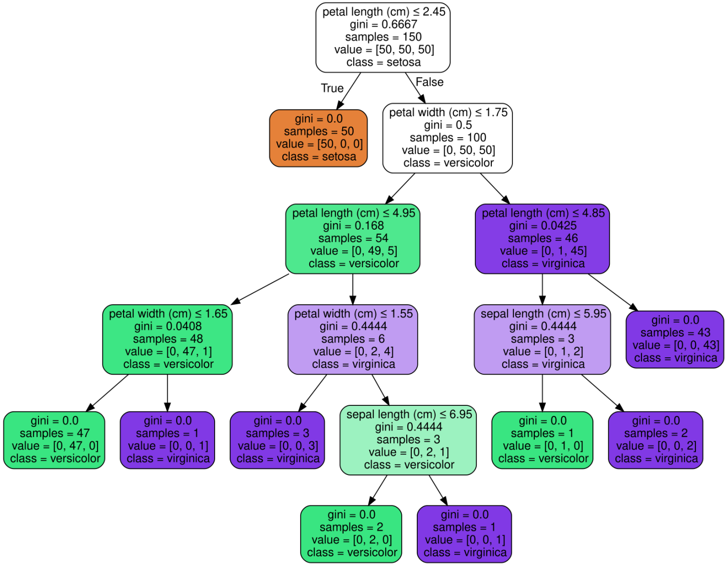


Soft margins

## SVM summary

- Allows for kernels (linear, polynomial, Gaussian, etc.) $\rightarrow$ ideal for non-linearly separable data
- Can be tuned for "more robust inference" vs "more precise inference of boundary"
- Efficient when predicting: complexity proportional to number of support vectors.

## Decision tree



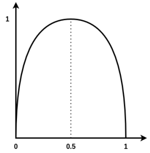
## Decision tree

- Can be used for classification or regression
- Simple algorithm: recursively decide on a variable to split that minimizes the expectation of a loss in the subsequent leaves (regression: variance, classification: entropy of the outcome)

## Decision tree example

Classification into two classes using entropy loss:

$$E = -P(\text{class } 1)\log(P(\text{class } 1)) - P(\text{class } 2)(\log P(\text{class } 2))$$



High entropy if "data is mixed".

**Example**

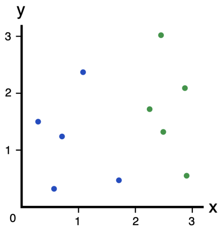
In a dataset with 20 elements, 14 are class 1 and 6 are class 2, the entropy can be computed as:

$$E = -\frac{14}{20}\log(\frac{14}{20}) - \frac{6}{20}\log(\frac{6}{20}) = 0.880$$

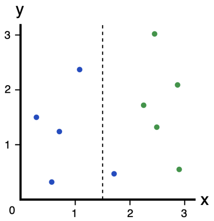
## Decision tree example

Information Gain (IG) is the decrease in entropy after the dataset is split:

$$IG = E - E_{\text{split}}$$



The Dataset



An Imperfect Split

Before split (5 blue, 5 green): $E = -0.5\log(0.5) - 0.5\log(0.5) = 1.$

After the split: $E_{left} = 0,\ E_{right} = -\frac{1}{6}\log(\frac{1}{6}) - \frac{5}{6}\log(\frac{5}{6}) = 0.65$

$$E_{split} = 0.4 \cdot E_{left} + 0.6 \cdot E_{right} = 0.39$$

$$IG = 1 - 0.39 = 0.61$$

## Decision tree

- Can be used for classification or regression
- Simple algorithm: recursively decide on a variable to split that minimizes the expectation of a loss in the subsequent leaves (regression: variance, classification: entropy / Gini impurity)

**Issue**

Imagine that the splits are partitioning the data in a half at each step of the inference algorithm. Can you foresee any issue?

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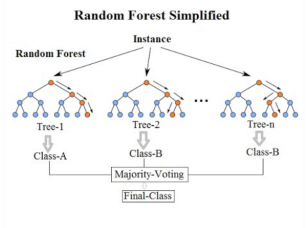
Possible way out: random forests.

## Random forest

Simple idea:

- bootstrap the training set and learn a tree on each bootstrapped set
- for a prediction, run all decision tree and aggregate with a majority vote



For free, we get also uncertainty measure by looking at the variance of the predictions in each decision tree.