

Statistics and Learning

Lecturers (alphabetic order):

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Lecture 7/9

Classification: logistic regression. Some models for supervised learning

Course objectives

- ▶ Classification using logistic regression
- ▶ Performance metrics for classifiers
- ▶ Prediction with decision trees
- ▶ Prediction with neural networks

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Lecture outline

1 – Some general notions about classification

2 – Logistic regression [classification]

3 – Decision trees [regression + classification]

4 – Neural networks [regression + classification]

5 – Standard exercices (with solutions)

6 – Appendices

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1.1 – Introduction

1.2 – Loss functions and associated optimal classifiers

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Mathematical framework and objectives

Notations

- ▶ $(X_1, Y_1), \dots, (X_n, Y_n) \stackrel{\text{iid}}{\sim} P^{X,Y}$
- ▶ $P^{X,Y}$: unknown distribution on $\mathcal{X} \times \mathcal{Y}$
- ▶ $\mathcal{X} \subset \mathbb{R}^p$, $\mathcal{Y} = \{0, 1, \dots, K-1\}$
- ▶ unless stated otherwise: $K = 2$ (**binary classification**)

Objectives

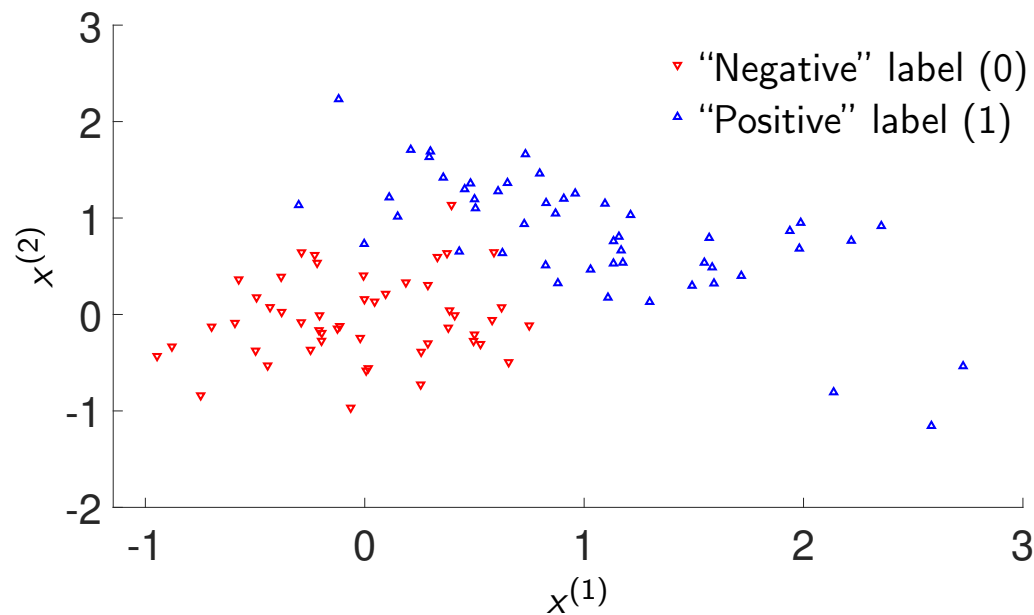
Construct a (good) prediction function $h : x \mapsto \{0, 1\}$.

Synonyms: **classification function**, or “classifier”.

Objectives of this section

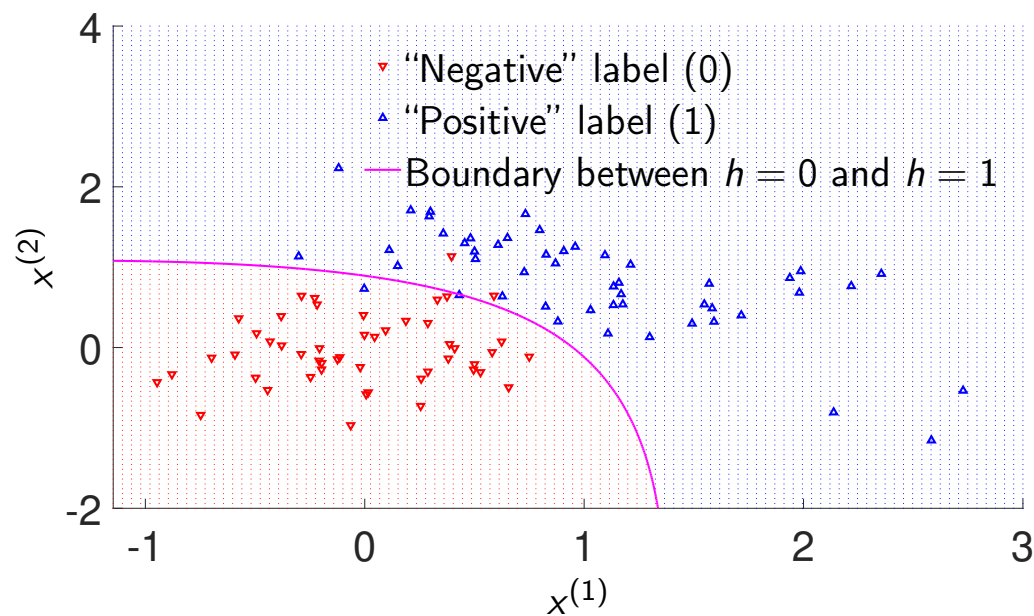
- ▶ introduction to the **logistic regression** method
- ▶ definition of relevant **risk measures** for classification

Example with two explanatory variables ($p = 2$)



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A taste of things to come: a possible classifier



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Reminder: loss function and risk

Definition: risk (generalization error)

Given a loss function $L : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$ and a prediction function $h : \mathcal{X} \rightarrow \mathcal{Y}$, the **risk**, or **generalization error**, is defined as :

$$R(h) = \mathbb{E} (L(Y, h(X))),$$

where the expectation is with respect to (X, Y) .



This risk **depends on the unknown distribution**:

$$R(h) = \iint_{\mathcal{X} \times \mathcal{Y}} L(y, h(x)) \mathbf{P}^{X,Y}(\mathrm{d}x, \mathrm{d}y).$$

Soft and hard classifiers

Consider a problem with two classes: $\mathcal{Y} = \{0, 1\}$.

Definition: hard classifier

A **hard classifier** is a measurable function $h : \mathcal{X} \rightarrow \mathcal{Y}$ from the instance space to the label space.

Remark: special case of a prediction function, cf. Lecture 6.

Definition: soft classifier

A **soft classifier** is a measurable function $h : \mathcal{X} \rightarrow [0, 1]$ from the instance space to $[0, 1]$.

Given a soft classifier $h : \mathcal{X} \rightarrow [0, 1]$, we can construct a family of hard classifiers, of the form $x \mapsto \mathbb{1}_{h(x) \geq \delta}$, for $\delta \in [0, 1]$.

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Commonly used loss functions

Definition: 0/1 loss for hard classification

$$\begin{aligned} L : \mathcal{Y} \times \mathcal{Y} &\rightarrow \mathbb{R}_+ \\ (y, \tilde{y}) &\mapsto L(y, \tilde{y}) = \mathbb{1}_{y \neq \tilde{y}}. \end{aligned}$$

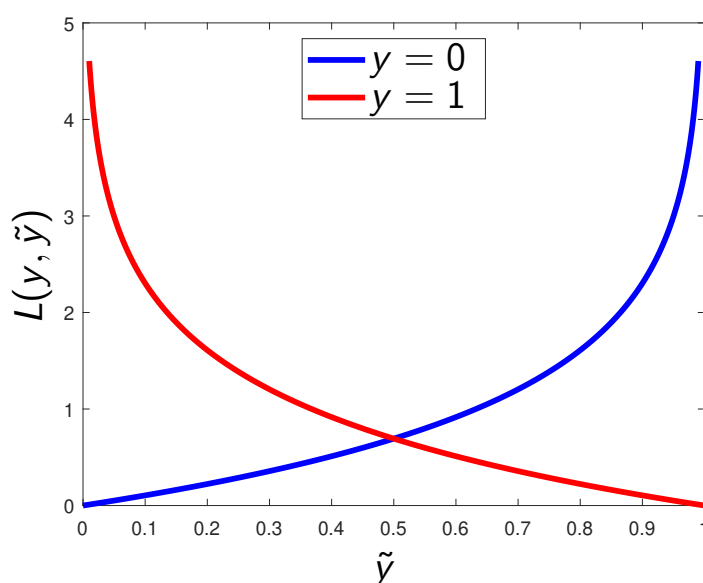
► $R(h) = \mathbb{P}(Y \neq h(X))$ is the **probability of misclassification**.

Definition: Logarithmic loss for soft classification

$$\begin{aligned} L : \mathcal{Y} \times [0, 1] &\rightarrow \mathbb{R}_+ \\ (y, \tilde{y}) &\mapsto L(y, \tilde{y}) = \begin{cases} -\ln(\tilde{y}) & \text{if } y = 1, \\ -\ln(1 - \tilde{y}) & \text{if } y = 0. \end{cases} \end{aligned}$$

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Commonly used loss functions (cont'd)



Remark: for both loss functions,

- ▶ $L(y, \tilde{y}) \geq 0$,
- ▶ $L(y, \tilde{y}) = 0 \Leftrightarrow \tilde{y} = y$.

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Optimal classification functions

Proposition

$h : \mathcal{X} \rightarrow \mathcal{Y}$ is optimal for the **0/1 loss** iff, P^X -ae,

- ▶ $h(x) = 1$ when $P(Y = 1 | X = x) > \frac{1}{2}$,
- ▶ $h(x) = 0$ when $P(Y = 1 | X = x) < \frac{1}{2}$.

with the notation $P(A | X = x) = \mathbb{E}(\mathbb{1}_A | X = x)$.

proof: see PC 7

For instance, $x \mapsto \mathbb{1}_{P(Y=1|X=x) \geq \frac{1}{2}}$ is optimal.

Remark: a more general formula can be proved for an asymmetric loss ($L(0, 1) \neq L(1, 0)$). See PHC's lecture notes.

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Optimal classification functions (cont'd)

Proposition

$h : \mathcal{X} \rightarrow [0, 1]$ is optimal for the **logarithmic loss** iff, P^X -ae,

$$h(x) = P(Y = 1 \mid X = x).$$

proof: exercise 1

Remark: since Y takes its values in $\{0, 1\}$, we have:

$$P(Y = 1 \mid X = x) = \mathbb{E}(Y \mid X = x).$$

☞ soft classification + logarithmic loss \approx **regression**.

(Hence the name of the method that we are about to study!)

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Confusion matrix & associated definitions

	Truth Negative (N)	Truth Positive (P)
Prediction Negative	True Negative (TN)	False Negative (FN)
Prediction Positive	False Positive (FP)	True Positive (TP)

True Positive Rate

$$TPR = \frac{TP}{P} = \frac{TP}{TP + FN}$$

(also called **sensitivity**)

True Negative Rate

$$TNR = \frac{TN}{N} = \frac{TN}{TN + FP}$$

(also called **specificity**)

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Confusion matrix & associated definitions (cont'd)

Alternative terminology, from the field of signal processing:

- ▶ $1 - TPR$ is the **miss rate** (false negative rate)
- ▶ $1 - TNR$ is the **false alarm rate** (false positive rate)

Applications to soft classifiers

- ▶ Reminder: to any given soft classifier h , we can associate a family of hard classifiers

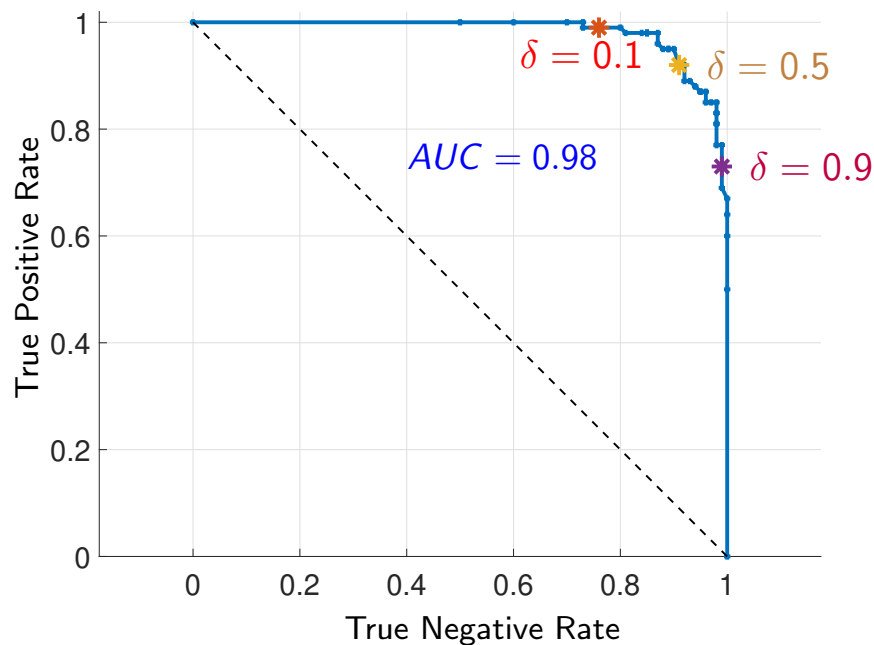
$$h_\delta : x \mapsto \mathbb{1}_{h(x) \geq \delta}, \quad \delta \in [0, 1].$$

- ▶ The value of δ impacts the TNR/TPR trade-off
 - ▶ when $\delta \nearrow$, **TNR** \nearrow , and **TPR** \searrow

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ROC curve (Receiver Operating Characteristic)

- ▶ a tool for **decision support** (choice of δ)
- ▶ a tool useful for **classifier comparison**
- ▶ associated definition: **AUC** = Area Under the Curve



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 - 2.1 – A linear model for soft classification
 - 2.2 – Training: selecting the coefficients
 - 2.3 – Back to the introductory example
 - 2.4 – Extensions
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A linear model for soft classification

Consider a (binary) **classification** problem

► $\mathcal{X} \subset \mathbb{R}^p$, $\mathcal{Y} = \{0, 1\}$.

Choose the **logarithmic loss**:

► the goal is to approximate the optimal soft classifier

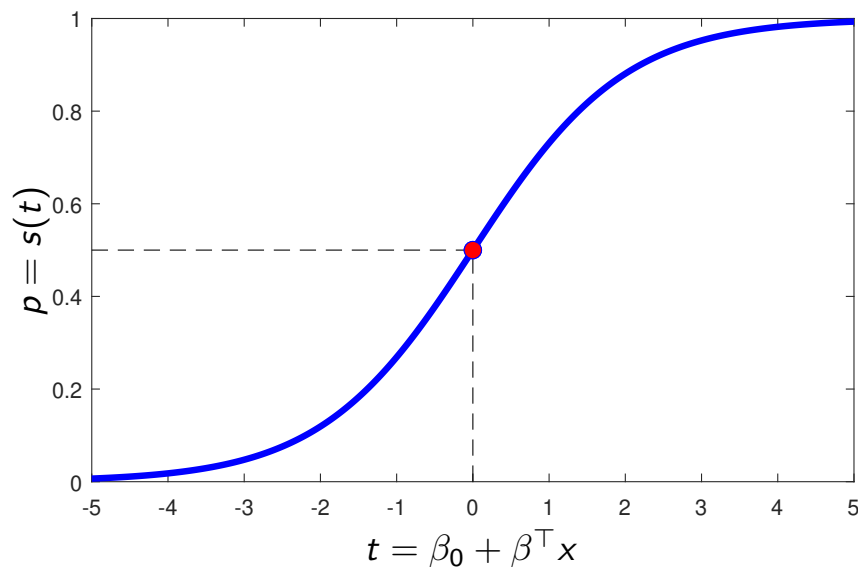
$$h^*(x) = \mathbb{P}(Y = 1 \mid X = x).$$

Logistic regression consists in using classifiers of the form

$$h(x) = s\left(\beta_0 + \beta^\top x\right),$$

with $\beta_0 \in \mathbb{R}$, $\beta \in \mathbb{R}^p$, and $s(t) = e^t / (1 + e^t)$ the **logistic function**.

The logistic function



▮▮▮ defines a correspondence: $\beta_0 + \beta^\top x \in \mathbb{R} \longleftrightarrow \text{proba } p \in (0, 1)$

Also known as the **sigmoid function**.

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A linear model for soft classification (cont'd)

Equivalently,

$$\text{logit}(h(x)) = \beta_0 + \beta^\top x$$

with

$$\begin{aligned} \text{logit} : (0, 1) &\rightarrow \mathbb{R} \\ p &\mapsto \ln\left(\frac{p}{1-p}\right) \end{aligned}$$

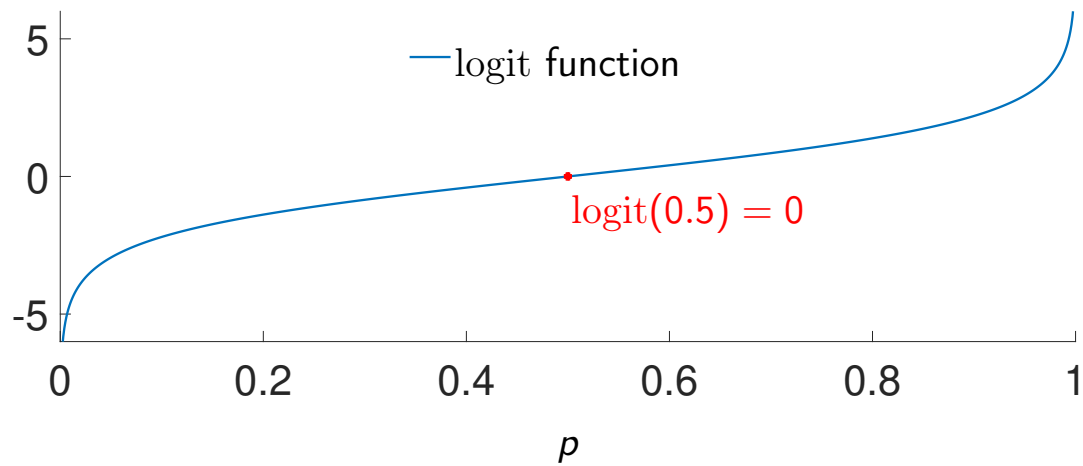
the **logit function**.

Properties

- ▶ The **logistic function** s is a strictly increasing, C^∞ bijection from \mathbb{R} to $(0, 1)$.
- ▶ The **logit function** is the inverse function: it is strictly increasing and C^∞ from $(0, 1)$ to \mathbb{R} .

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The logit function



⇒ defines a correspondence: proba $p \in (0, 1) \longleftrightarrow \beta_0 + \beta^\top x \in \mathbb{R}$

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From soft to hard classification

Given a **soft classifier** of the form

$$h(x) = s(\beta_0 + \beta^\top x),$$

and a **decision threshold** $\delta \in [0, 1]$, we set:

$$h_\delta(x) = \mathbb{1}_{h(x) \geq \delta}.$$

⇒ h_δ separates the classes in \mathcal{X} by an **affine hyperplane**:

$$h_\delta(x) = 1 \iff \beta_0 + \beta^\top x \geq \text{logit}(\delta)$$

For the 0/1 loss, the value $\delta = \frac{1}{2}$ is generally used.

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Minimization of the empirical risk

Simplification of notations: $x \rightarrow \begin{pmatrix} 1 \\ x \end{pmatrix}$ and $\beta \rightarrow \begin{pmatrix} \beta_0 \\ \beta \end{pmatrix}$

$$\Rightarrow h(x) = \frac{\exp(\beta^\top x)}{1 + \exp(\beta^\top x)}$$

The parameter β is selected using **empirical risk minimization**..:

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \mathbb{R}^{p+1}} \frac{1}{n} \sum_{i=1}^n L(Y_i, h(X_i)),$$

where L denotes the **logarithmic loss**.

Minimization of the empirical risk (cont'd)

Equivalence between empirical risk minimization and MLE

$$\sum_{i=1}^n L(y_i, h(x_i)) = -\ln \left(\underbrace{\prod_{i=1}^n (h(x_i))^{y_i} (1 - h(x_i))^{1-y_i}}_{\text{likelihood } \mathcal{L}(\beta; \underline{X}, \underline{Y})} \right)$$

Interpretation: $\hat{\beta}$ is the **MLE of the parametric model**

$$Y_i | X_i \stackrel{\text{iid}}{\sim} \text{Ber}(h(X_i)), \quad h(x) = \frac{\exp(\beta^\top x)}{1 + \exp(\beta^\top x)}, \quad \beta \in \mathbb{R}^{p+1}.$$

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Log-likelihood

Log-likelihood

(see PC)

$$\begin{aligned} \ell(\beta) &= \ln \mathcal{L}(\beta; \underline{X}, \underline{Y}) \\ &= \sum_{i=1}^n \left\{ Y_i \beta^\top X_i - \ln \left(1 + \exp(\beta^\top X_i) \right) \right\} \end{aligned}$$

Maximization of ℓ

Using a numerical **optimization algorithm**

► for instance, the Newton-Raphson algorithm

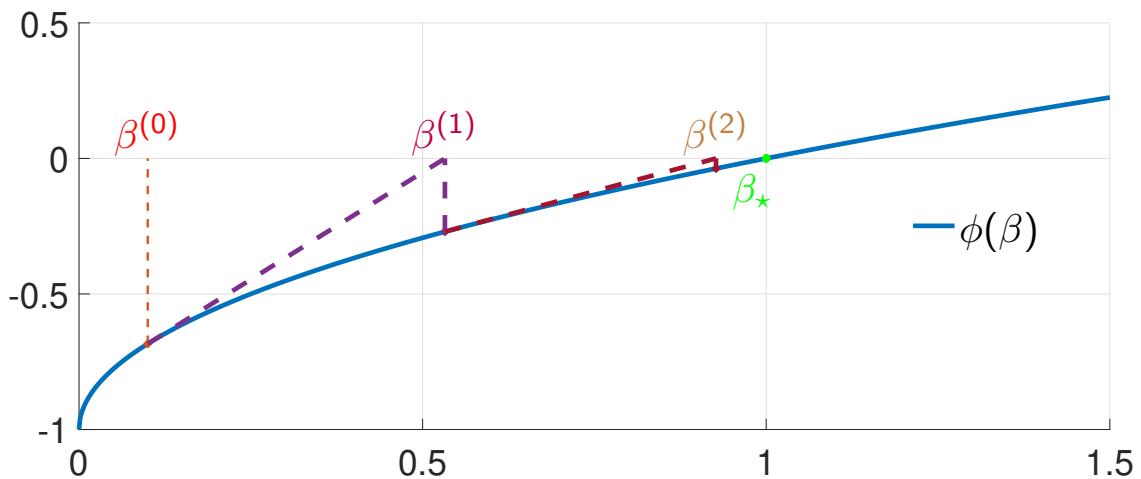
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Reminder: Newton-Raphson algorithm in one dimension

Let $\phi : \mathbb{R} \rightarrow \mathbb{R}$. We want β that satisfies $\phi(\beta) = 0$

Newton-Raphson algorithm is iterative:

- ▶ initialization: $\beta^{(0)}$
- ▶ iteration: $\beta^{(k+1)} = \beta^{(k)} - \frac{\phi(\beta^{(k)})}{\phi'(\beta^{(k)})}$



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Maximization of ℓ using the Newton-Raphson method

Same algorithm but now in dimension $p + 1$, with:

- ▶ $\phi \rightarrow \nabla_{\beta} \ell$
- ▶ $\phi' \rightarrow \nabla_{\beta}^2 \ell$

The iteration follows:

$$\beta^{(k+1)} = \beta^{(k)} - \left[\nabla_{\beta}^2 \ell \left(\beta^{(k)} \right) \right]^{-1} \nabla_{\beta} \ell \left(\beta^{(k)} \right)$$

Under the following conditions:

- ▶ $\nabla_{\beta}^2 \ell (\cdot)$ is Lipschitz continuous,
- ▶ $\nabla_{\beta}^2 \ell \left(\beta^{(0)} \right)$ is invertible
- ▶ $h_0 = \left[\nabla_{\beta}^2 \ell \left(\beta^{(0)} \right) \right]^{-1} \nabla_{\beta} \ell \left(\beta^{(0)} \right)$ small enough[†],

the algorithm converges to a point β^* such that $\nabla_{\beta} \ell (\beta^*) = 0$.

[†] cf. "Kantorovich theorem" on wikipedia for a more precise statement

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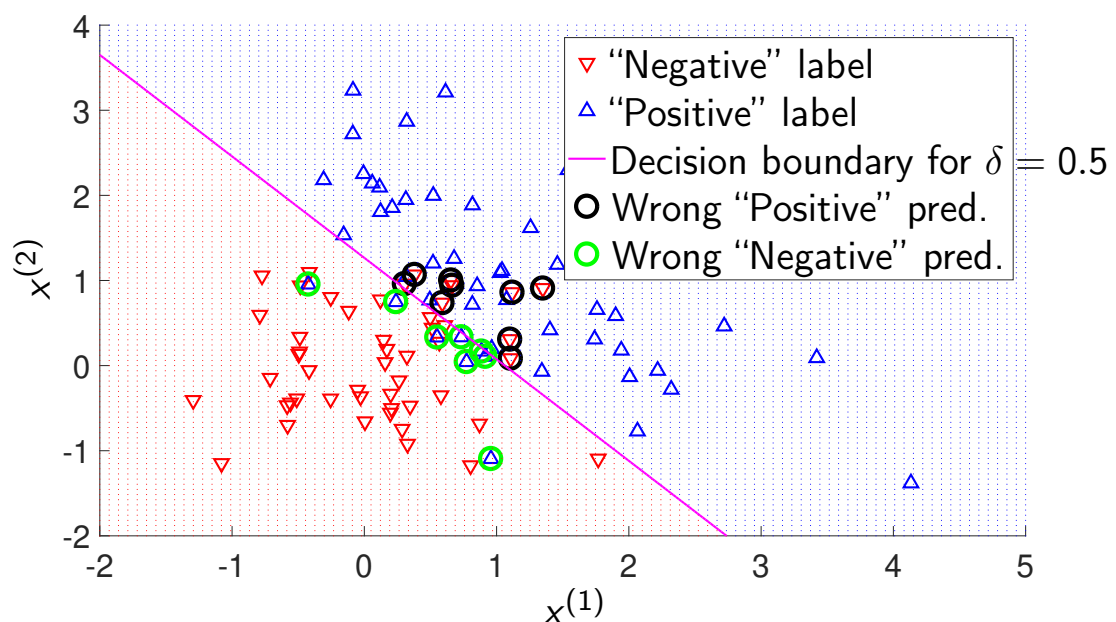
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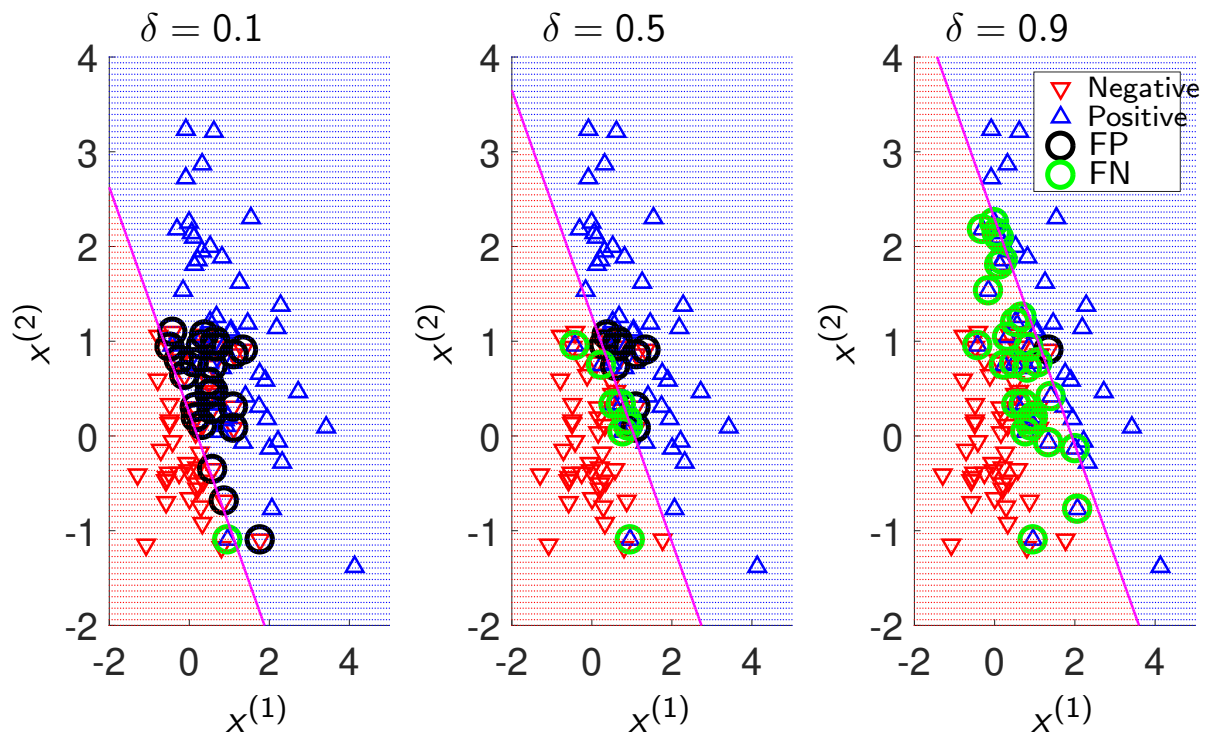
LR performed on the example with 2 explanatory variables



Prediction errors:

- ▶ "Negative" examples predicted as "Positive"
- ▶ "Positive" examples predicted as "Negative"

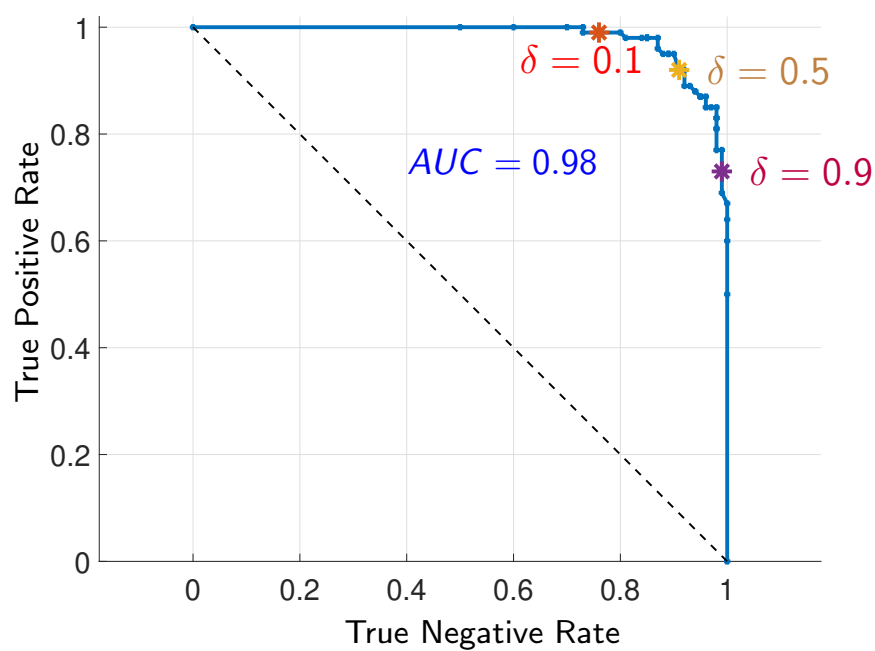
Influence of δ



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ROC curve (Receiver Operating Characteristic)

- ▶ a tool for **decision support** (choice of δ)
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Extension: large number of variables

How to handle the case where p is large

The log-likelihood is **penalized**:

► $L_1 : \hat{\beta} = \arg \max_{\beta} (\ell(\beta) - \lambda \|\beta\|^2)$

► $L_2 : \hat{\beta} = \arg \max_{\beta} (\ell(\beta) - \lambda \|\beta\|_1)$

⇒ see Lecture 8

p is “large” if $p \gg n$, or even simply $p \approx n$

Extension: more than two classes

Multiclass classification

Let $\{0, 1, \dots, K - 1\}$ be the set of labels (classes), $K \geq 3$.

One class is chosen as the reference class and $K - 1$ binary logistic regressions are performed (here class “0” was chosen):

$$\begin{cases} \ln \left(\frac{P(Y=\mathbf{1}|X=x)}{P(Y=\mathbf{0}|X=x)} \right) &= \beta_{\mathbf{1},0} + \beta_{\mathbf{1}}^T x \\ \vdots \\ \ln \left(\frac{P(Y=\mathbf{K-1}|X=x)}{P(Y=\mathbf{0}|X=x)} \right) &= \beta_{\mathbf{K-1},0} + \beta_{\mathbf{K-1}}^T x \end{cases}$$

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Binary classification: spam detection

Data collected over 4601 e-mails

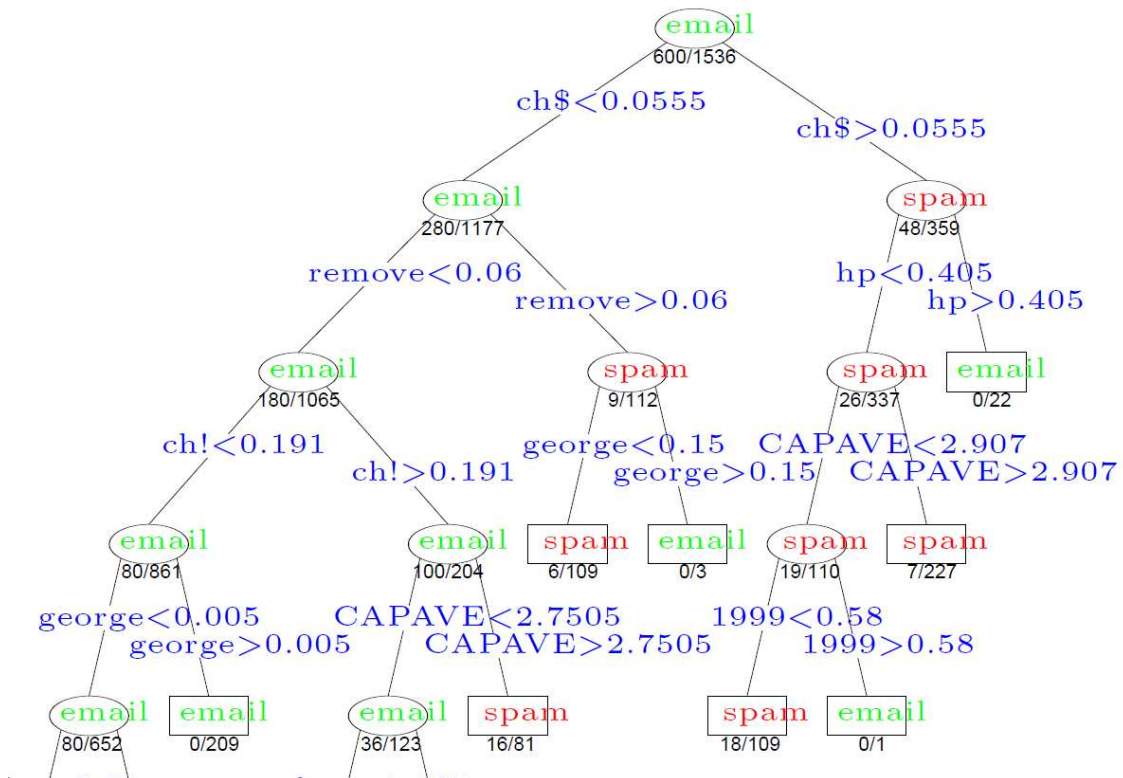
- ▶ explanatory variables: relative freq. of 57 of the most used words
- ▶ variable to be explained: label “Spam” or “Email”
 - ➡ **categorical** variable (binary in this example)

TABLE 1.1. Average percentage of words or characters in an email message equal to the indicated word or character. We have chosen the words and characters showing the largest difference between spam and email.

	george	you	your	hp	free	hpl	!	our	re	edu	remove
spam	0.00	2.26	1.38	0.02	0.52	0.01	0.51	0.51	0.13	0.01	0.28
email	1.27	1.27	0.44	0.90	0.07	0.43	0.11	0.18	0.42	0.29	0.01

TABLE 9.3. Spam data: confusion rates for the 17-node tree (chosen by cross-validation) on the test data. Overall error rate is 9.3%.

True	Predicted	
	email	spam
email	57.3%	4.0%
spam	5.3%	33.4%

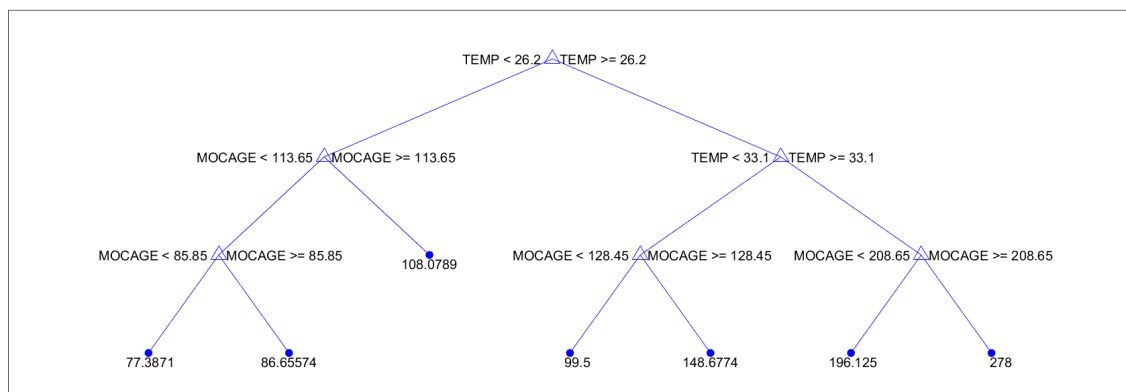


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Regression tree: "Ozone" example

Simplified example (for the sake of visualization)

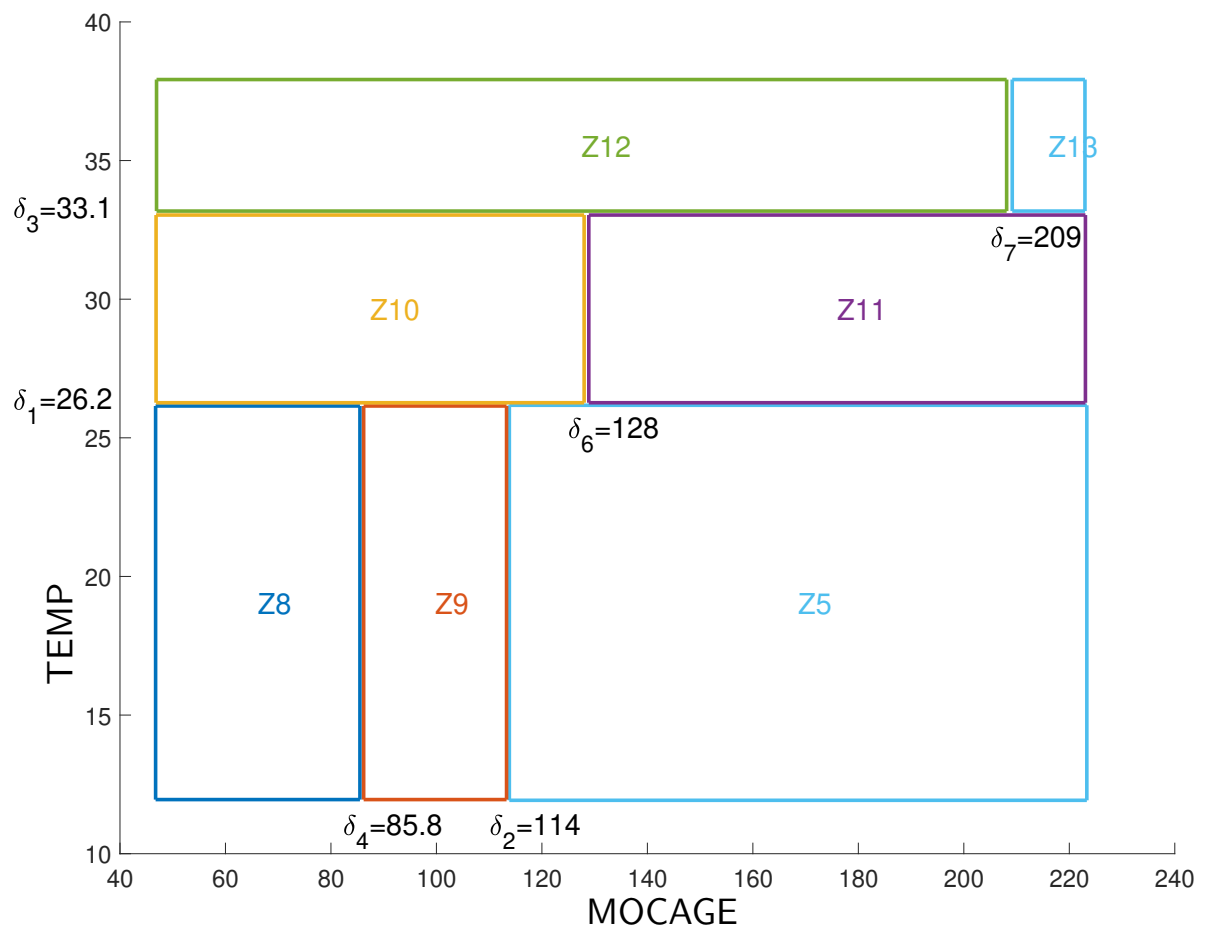
- ▶ predict variable O3 (**quantitative** variable)
- ▶ from variables MOCAGE and TEMP



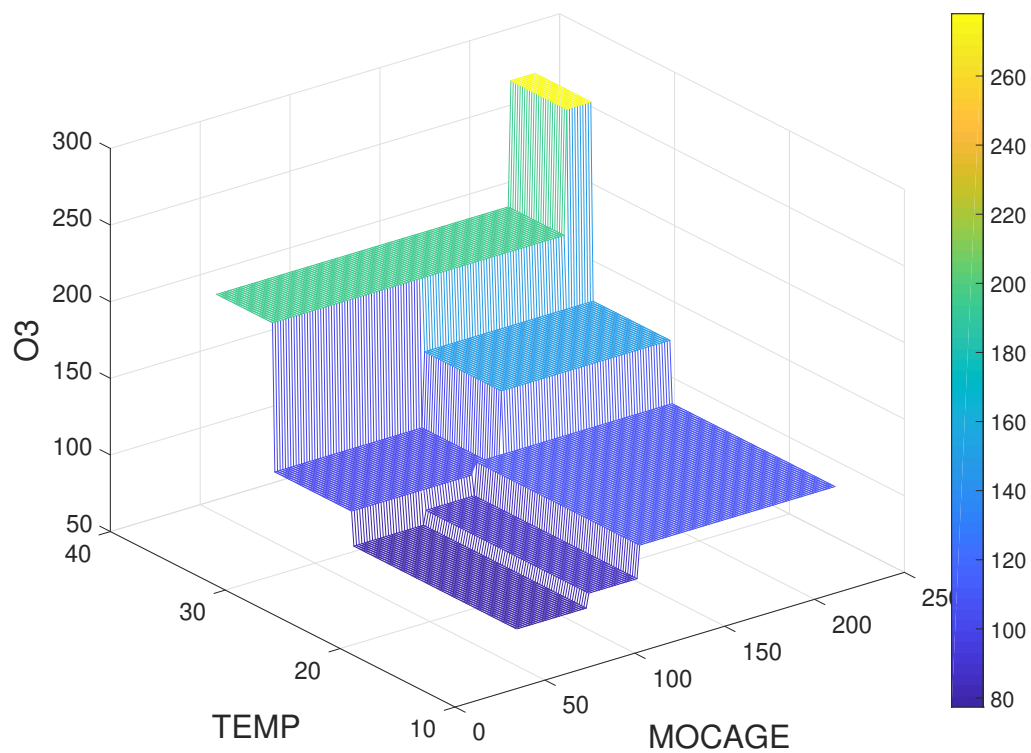
Vocabulary. When the variable to be explained is

- ▶ **quantitative** → **regression tree**
- ▶ **categorical** → **classification tree**

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Regression tree: "Ozone" example



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Recursive partitioning: general principle

Objectives

Construct a partition of \mathcal{X} from the data $(\underline{X}, \underline{Y})$.

Principle: **iterative** construction of a sequ. $(\mathcal{P}_m)_{m \geq 1}$ of partitions,

► $\mathcal{P}_m = \{Z_1^{(m)}, \dots, Z_m^{(m)}\}$, where partition \mathcal{P}_m contains m subsets.

Initialization: $\mathcal{P}_1 = \{\mathcal{X}\}$.

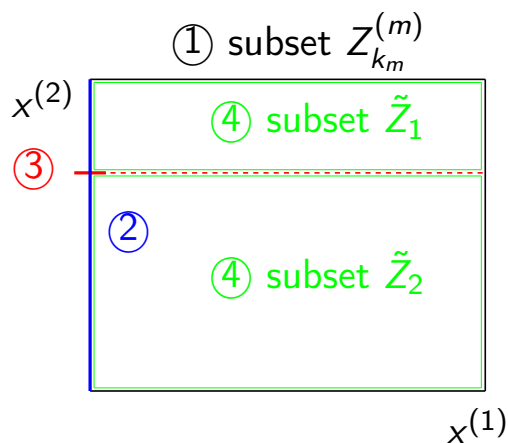
$\mathcal{P}_m \rightarrow \mathcal{P}_{m+1}$: **split** a subset $Z_{k_m}^{(m)}$ **along one of the variables**:

► $\tilde{Z}_1 = Z_{k_m}^{(m)} \cap \{x \text{ such that } x^{(j_m)} \leq \delta_m\}$

► $\tilde{Z}_2 = Z_{k_m}^{(m)} \cap \{x \text{ such that } x^{(j_m)} > \delta_m\}$

(the index j_m and the threshold δ_m still have to be specified)

An example with $p = 2$



Iteration $\mathcal{P}_m \rightarrow \mathcal{P}_{m+1}$:

- ▶ ① subset $Z_{k_m}^{(m)} \in \mathcal{P}_m$
- ▶ ② variable $x^{(j_m)}$ (here $j_m = 2$)
- ▶ ③ threshold δ_m
- ▶ ④ construction of \tilde{Z}_1 and \tilde{Z}_2

After splitting $Z_{k_m}^{(m)}$, we get:

$$\mathcal{P}_{m+1} = \mathcal{P}_m \cup \{\tilde{Z}_1, \tilde{Z}_2\} \setminus \{Z_{k_m}^{(m)}\}$$

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Choice of k_m , j_m and δ_m

Let $D(Z)$ be a measure of the **heterogeneity** of a subset Z .

Example (for a quantitative label y)

$$D(Z) = \sum_{i \in Z} (y_i - \bar{y}_Z)^2$$

where \bar{y}_Z is the empirical mean computed over Z .

k_m , j_m and δ_m are jointly chosen in such a way that

$D(Z_{k_m}^{(m)}) - D(\tilde{Z}_1) - D(\tilde{Z}_2)$ is as large as possible

⇒ largest reduction of heterogeneity

(Recall that \tilde{Z}_1 and \tilde{Z}_2 are the subsets obtained by splitting $Z_{k_m}^{(m)}$)

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Piecewise constant prediction function

Decision trees define a **piecewise constant prediction function** on the elements of the partition:

$$h_{\beta}(x) = \sum_{k=1}^m \beta_k \mathbb{1}_{Z_k^{(m)}}(x).$$

Remark: for a given partition, this is a **linear model** with respect to the m variables $\mathbb{1}_{Z_k^{(m)}}(x)$.

Estimation of the coefficients

Principle: to estimate $\beta^{(m)} = (\beta_1^{(m)}, \dots, \beta_m^{(m)})$,

- ▶ choose a **loss function** $L(y, h_\beta(x))$,
- ▶ then **minimize the empirical risk**.

Simplification:

$$\begin{aligned}\min_{\beta} \hat{\mathcal{R}}(h_{\beta}) &= \min_{\beta} \sum_{i=1}^n L(y_i, h_{\beta}(x_i)) \\ &= \min_{\beta} \sum_{k=1}^m \sum_{i \in Z_k^{(m)}} L(y_i, \beta_k) \\ &= \sum_{k=1}^m \min_{\beta_k} \sum_{i \in Z_k^{(m)}} L(y_i, \beta_k)\end{aligned}$$

Consequence: $\forall k, \hat{\beta}_k^{(m)} = \arg \min_{\beta_k} \sum_{i \in Z_k^{(m)}} L(y_i, \beta_k)$.

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Two important special cases

Regression with the **quadratic loss**

$$\hat{\beta}_k^{(m)} = \operatorname{argmin}_{\beta_k} \sum_{i \in Z_k^{(m)}} (y_i - \beta_k)^2 = \bar{y}_{Z_k^{(m)}}$$

Binary classification with the **logarithmic loss**

Soft classification:

$$\begin{aligned}\hat{\beta}_k^{(m)} &= \operatorname{argmin}_{\beta_k \in [0,1]} \sum_{i \in Z_k^{(m)}} (-y_i \ln(\beta_k) - (1 - y_i) \ln(1 - \beta_k)) \\ &= \frac{1}{\operatorname{card}(Z_k^{(m)})} \cdot \operatorname{card}\left(i \in Z_k^{(m)} \text{ such that } y_i = 1\right)\end{aligned}$$

Hard classification: threshold at $\delta = \frac{1}{2}$ (cf. logistic regression).

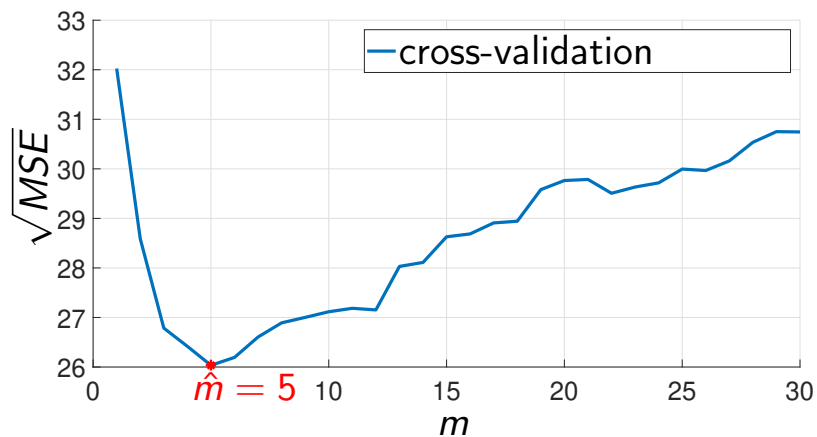
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Choosing the size m of the partition

- ▶ m can either be given beforehand (\sim prior knowledge)
- ▶ or estimated by **cross-validation**.

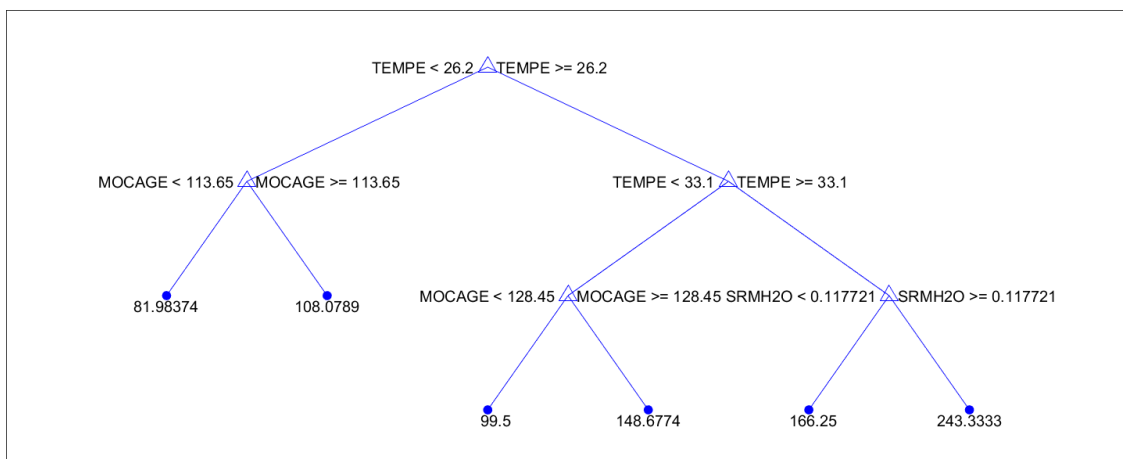
“Ozone” example

- ▶ Regression of O3 with $p = 7$ explanatory variables
- ▶ m is chosen by leave-one-out cross-validation



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Regression tree: “Ozone” example



```
1 if TEMPE<26.2 then node 2 elseif TEMPE>=26.2 then node 3 else 103.433
2 if MOCAGE<113.65 then node 4 elseif MOCAGE>=113.65 then node 5 else 88.1429
3 if TEMPE<33.1 then node 6 elseif TEMPE>=33.1 then node 7 else 153.673
4 fit = 81.9837
5 fit = 108.079
6 if MOCAGE<128.45 then node 8 elseif MOCAGE>=128.45 then node 9 else 138.59
7 if SRMH2O<0.117721 then node 10 elseif SRMH2O>=0.117721 then node 11 else 212.5
8 fit = 99.5
9 fit = 148.677
10 fit = 166.25
11 fit = 243.333
```

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More trees...

Disadvantages of decision trees

- ▶ high sensitivity to the sample $(\underline{x}, \underline{y})$
- ▶ piecewise constant prediction on each subset (by construct.)
(not satisfactory if the optimal prediction function is smooth)

Extensions

- ▶ aggregation of decisions tree models
 - ▮▮▮ ➔ **Random forests**
- ▶ weighted sum of weak classifiers
 - ▮▮▮ ➔ **Boosting** (AdaBoost)

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The (multipolar) biological neuron: axons, dendrites...

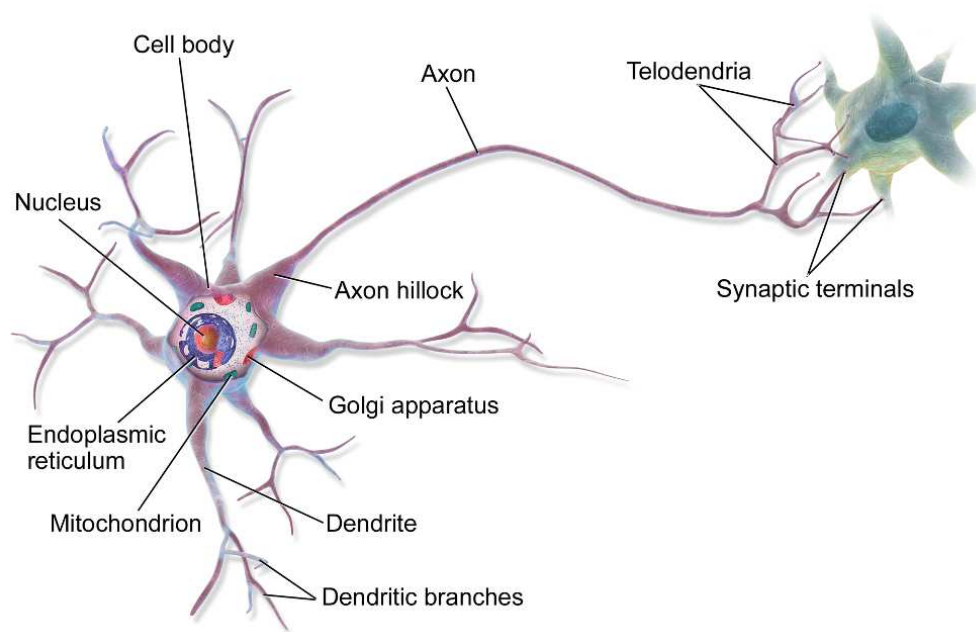


Image: Bruce Blaus, <https://commons.wikimedia.org>, CC BY 3.0

"A multipolar neuron is a type of neuron that possesses a single axon and many dendrites (and dendritic branches), allowing for the integration of a great deal of information from other neurons." (https://fr.wikipedia.org/wiki/Neurone_multipolaire)

The artificial neuron

Definition: neuron (McCulloch and Pitts, 1943)[†]

In statistical learning, a **neuron** with p variables (inputs) is a function, generally non-linear[‡], of the form

$$h(x) = \varphi(w x + b), \quad x \in \mathbb{R}^p,$$

where

- ▶ φ is an increasing $\mathbb{R} \rightarrow \mathbb{R}$ function;
- ▶ $w \in \mathbb{R}^{1 \times p}$, and $b \in \mathbb{R}$.

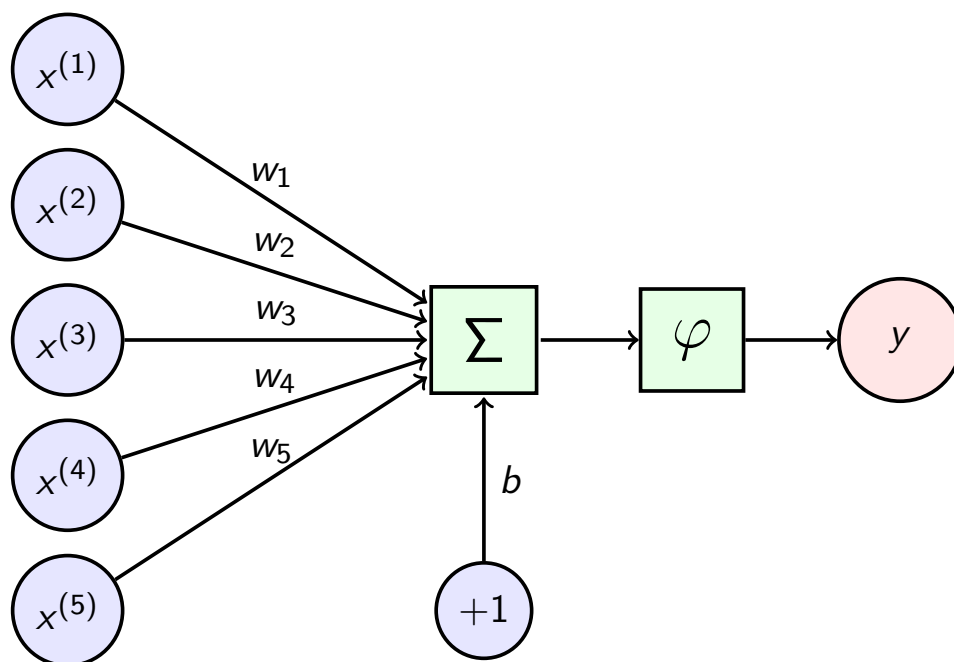
Vocabulary

- ▶ φ : **activation function**,
- ▶ w_1, \dots, w_p : **weights**,
- ▶ b : **bias** (nothing to do with the bias of an estimator).

[†] The original neuron of McCulloch & Pitts (1943) specifically used $\varphi = \text{sgn}$ as an activation function.

[‡] We will see later a situation where a linear neuron ($\varphi = \text{Id}$) is used.

The artificial neuron: illustration ($p = 5$)



Activation functions

Discontinuous activation functions (not recommended[†]):

- ▶ **Heaviside** function: $\varphi(v) = \mathbb{1}_{v \geq 0}$, or
- ▶ **sign** function: $\varphi(v) = \text{sgn}(v) = \mathbb{1}_{v > 0} - \mathbb{1}_{v < 0}$.

“S-shaped” functions, a.k.a. **sigmoids**:

- ▶ **logistic**[‡]: $\varphi(v) = \frac{1}{1+e^{-v}} = \frac{1}{2} + \frac{1}{2} \tanh\left(\frac{v}{2}\right)$, or
- ▶ **tanh**: $\varphi(v) = \tanh(v) = \frac{e^v - e^{-v}}{e^v + e^{-v}}$.

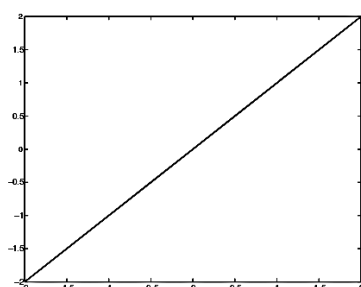
The **ReLU** (*Rectified Linear Unit*) function:

- ▶ $\varphi(v) = \max(0, v)$.

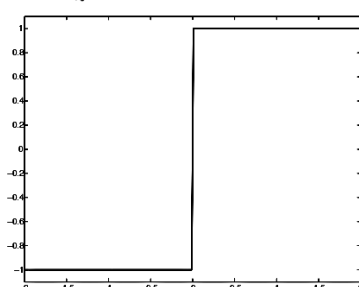
[†] Used in the oldest models, most notably the Rosenblatt's perceptron (1957), but abandoned since then because of their almost-everywhere zero gradient, which creates problems for optimization procedures.

[‡] The word “sigmoid” sometimes refers to this particular function.

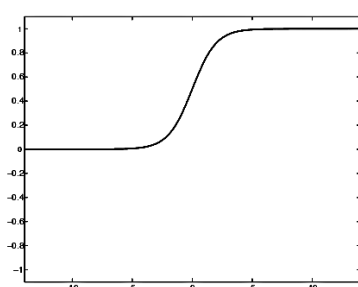
Activation functions (cont'd)



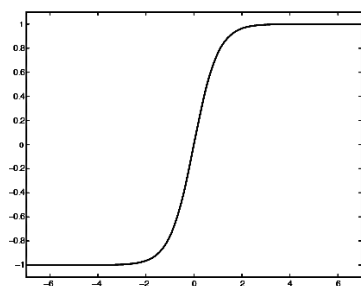
(a) Identity



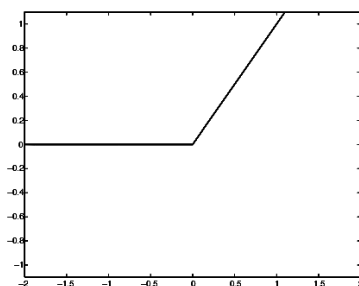
(b) Sign



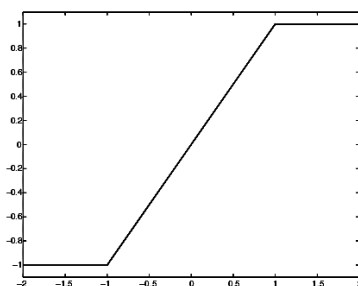
(c) Sigmoid



(d) Tanh



(e) ReLU



(f) Hard Tanh

Image: C. C. Aggarwal (2018). *Neural networks and Deep Learning*, Springer.

Remark: relation with logistic regression

Remark. With the **logistic activation function** (sigmoid),

$$y = \varphi(v) = \frac{1}{1 + e^{-v}} \quad \Leftrightarrow \quad v = \ln \left(\frac{y}{1 - y} \right).$$

Since $v = wx + b$, we recover for $h(x)$ the form of the **logistic regression predictor**.

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Multi-layer perceptron: definition

Let p, K be non-zero integers.

Definition: multi-layer perceptron[†] (MLP)

We call **multi-layer perceptron** with $M + 1$ layers, p variables (input) and K responses (output), any function $\mathbb{R}^p \rightarrow \mathbb{R}^K$ of the form

$$h = \left(\underline{\varphi}_M \circ g_M \right) \circ \cdots \circ \left(\underline{\varphi}_j \circ g_j \right) \circ \cdots \circ \left(\underline{\varphi}_1 \circ g_1 \right),$$

where[‡]

- ▶ $g_k : \mathbb{R}^{m_{k-1}} \rightarrow \mathbb{R}^{m_k}$ is **affine**,
- ▶ $\underline{\varphi}_k : \mathbb{R}^{m_k} \rightarrow \mathbb{R}^{m_k}$ represents the action coordinate by coordinate of an **increasing function** $\varphi_k : \mathbb{R} \rightarrow \mathbb{R}$.
- ▶ m_0, m_1, \dots, m_M : non-zero integers, $m_0 = p, m_M = K$.

[†] Rosenblatt's original perceptron (1957) did not include hidden layers ($M = 1$). It was using the activation function $h(x) = \text{sgn}(x)$ as McCulloch and Pitts (1943), and weights $w_j \in \{-1, +1, -\infty\}$.

[‡] there will be one exception this rule later ("softmax" layer)

Multi-layer perceptron: definition (cont'd)

Vocabulary: **layers** of variables

- ▶ $z_{[0]} = x$: input layer,
- ▶ $z_{[k]} = (\underline{\varphi}_k \circ g_k)(z_{[k-1]})$, $1 \leq k < M$: **hidden layers**,
- ▶ $z_{[M]} = y = (\underline{\varphi}_M \circ g_M)(z_{[M-1]})$: output layer.

Remark. Let us write

$$g_k(z_{[k-1]}) = W_k z_{[k-1]} + b_k.$$

Then, for all $j \in \{1, \dots, m_k\}$ we recognize a **neuron**:

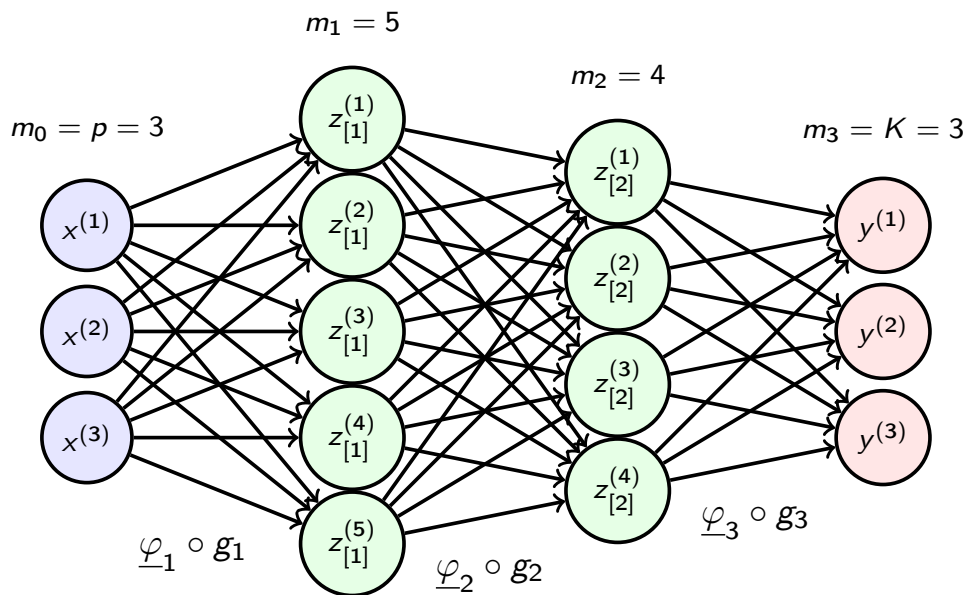
$$z_{[k]}^{(j)} = \varphi_k \left(w_{k,j} z_{[k-1]} + b_k^{(j)} \right),$$

where $w_{k,j} = e_j^\top W_k$ is the j -th row of W_k .

▮ Vocabulary: weights, bias, activation function.

Multi-layer perceptron: illustration

Example of a multi-layer perceptron with $p = 3$ inputs, $K = 3$ outputs, and two hidden layers of sizes $m_1 = 5$ and $m_2 = 4$.



Vocabulary: fully connected, feed-forward neural network

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Output layer: activation function

The output layer must be **adapted to the problem** at hand...

Regression. $\mathcal{Y} \subset \mathbb{R}$, or more generally \mathbb{R}^K .

- ▶ Perceptron with K outputs
- ▶ Activation function: $\varphi_M = \text{Id}$.
- ▶ Thus the last transformation $(\varphi_M \circ g_M)$ is **linear** (affine).

Classification. K classes, $\mathcal{Y} = [0, 1]^K$ ("soft" classification).

- ▶ Perceptron with K outputs, with $m_{M-1} = m_M = K$.
- ▶ Exception to the definition \Rightarrow the "**softmax**" layer:

$$z_{[M]}^{(j)} = \frac{\exp\left(z_{[M-1]}^{(j)}\right)}{\sum_{j'=1}^K \exp\left(z_{[M-1]}^{(j')}\right)}, \quad \sum_{j=1}^K z_{[M]}^{(j)} = 1.$$

Remark: alternatively, for *binary* classification, we can use a single output ($K = 1$ instead of $K = 2$) with the *logistic* function used as the activation function on the last layer.

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Training: loss functions and regularization

The most commonly used loss functions[†] are

- ▶ **regression**: the **quadratic loss**
 - ▶ $L(y, \tilde{y}) = (y - \tilde{y})^2$ for the single-output case,
 - ▶ $L(y, \tilde{y}) = \|y - \tilde{y}\|^2$ if $K > 1$.
- ▶ (soft) **classification**: the **logarithmic loss**
 - ▶ For all $j \in \{1, \dots, K\}$, we have $y^{(j)} \in \{0, 1\}$ and $\tilde{y}^{(j)} \in [0, 1]$.
 - ▶ $L(y, \tilde{y}) = -\sum_{j=1}^K y^{(j)} \ln(\tilde{y}^{(j)})$.

Nb parameters is high \Rightarrow **regularize** to avoid **over-fitting**

- ▶ **penalization**, for instance L^1 (LASSO) or L^2 (ridge);
- ▶ other (not covered): early stopping, drop out...

[†] for instance https://scikit-learn.org/stable/modules/neural_networks_supervised.html

Training: numerical optimization

We want to **minimize the empirical risk** (possibly penalized)

$$\hat{\mathcal{R}}_n(\theta) = \frac{1}{n} \sum_{i=1}^n L(Y_i, h_{\theta}(X_i)),$$

where θ denotes the parameters of the model (weights, biases).

⇒ **Numerical methods** are used to this end.

These methods use the **gradient of the criterion**. Two remarks:

- ▶ computational burden when n is large: random “**mini-batches**”
 - ⇒ **stochastic gradient** method (not covered);
- ▶ recursive computation of the **gradient of a composition of fcts**
 - ⇒ **back-propagation** method (not covered).

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Example: MNIST



70 000 images[†] of size 28×28 pixels (256 gray levels)

Problem: multi-class classification (10 classes);

training: 60 000 images / test: 10 000 images

Source: <http://yann.lecun.com/exdb/mnist/>

Example: MNIST

▣▶ see Jupyter / Python / Scikit-Learn notebook

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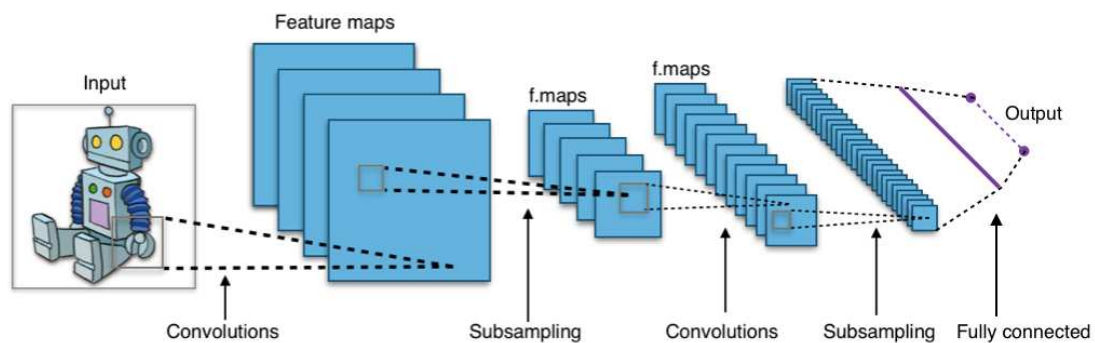
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Convolutional neural networks (CNNs)



Schematic diagram of a typical CNN

Image: Aphex34, <https://commons.wikimedia.org>, CC BY-SA 4.0

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Exercise 1 (Optimal classifier with the logarithmic loss)

▶ solution

Question

Show the proposition stated on ▶ slide 12 :

$h : \mathcal{X} \rightarrow [0, 1]$ is optimal for the **logarithmic loss** iff, P^X -ae,

$$h(x) = P(Y = 1 \mid X = x).$$

Exercise 2 (Multi-class logistic regression)

 solution

When the number of classes K is ≥ 3 , the classification problem is called **Multiclass**.

Let $\{0, 1, \dots, K - 1\}$ be the set of labels (classes), $K \geq 3$.

Binary logistic regression can be extended to multi-class classification by

- ▶ selecting a reference class (here, "0")
- ▶ performing $K - 1$ binary logistic regressions:

$$\begin{cases} \ln \left(\frac{P(Y=\mathbf{1}|X=x)}{P(Y=\mathbf{0}|X=x)} \right) &= \beta_{\mathbf{1},0} + \beta_{\mathbf{1}}^\top x \\ \vdots \\ \ln \left(\frac{P(Y=\mathbf{K-1}|X=x)}{P(Y=\mathbf{0}|X=x)} \right) &= \beta_{\mathbf{K-1},0} + \beta_{\mathbf{K-1}}^\top x \end{cases}$$

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Exercise 2 (Multi-class logistic regression (cont'd))

 solution

To simplify notation, we'll assume that the matrix of explanatory variables contains a constant vector and make the following change:

$$\beta_k \leftarrow (\beta_{k,0}, \beta_k)$$

Questions

- 1 Give the expression of $P(Y = k|X = x)$ from the vectors β_k ,
- 2 Deduce from 1. that the choice of reference class is arbitrary (it has no influence on the regression model),
- 3 Express the log-likelihood

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Solution of exercise 1

[back to questions](#)

The optimal classifier h^* minimizes $\mathbb{E}(L(Y, h(X)))$, where the expectation is taken over (X, Y) .

By conditioning, we have:

$$\mathbb{E}_{(X,Y)}(L(Y, h(X))) = \mathbb{E}_X(\mathbb{E}_{Y|X}(L(Y, h(X))|X))$$

Thus:

$$\begin{aligned} h^* &= \operatorname{argmin}_h \mathbb{E}(L(Y, h(X))) \\ &\quad \updownarrow \\ h^*(x) &= \operatorname{argmin}_{t \in \mathcal{Y}} \underbrace{\mathbb{E}(L(Y, t) \mid X = x)}_{\mathcal{J}(t)} \quad \mathbb{P}^X\text{-pp.} \end{aligned}$$

With the logarithmic loss:

$$\begin{aligned}
 \mathcal{J}(t) &= \mathbb{E}_{Y|X}(L(Y, t)|X = x) \\
 &= \mathbb{P}(Y = 1|X = x)L(1, t) + \mathbb{P}(Y = 0|X = x)L(0, t) \\
 &= \mathbb{P}(Y = 1|X = x)(L(1, t) - L(0, t)) + L(0, t) \\
 &= \mathbb{P}(Y = 1|X = x)(-\ln(t) + \ln(1 - t)) - \ln(1 - t)
 \end{aligned}$$

The minimization of $\mathcal{J}(t)$ is achieved by examining the sign of the derivative of $\mathcal{J}(t)$:

$$\begin{aligned}
 \mathcal{J}'(t) &= \mathbb{P}(Y = 1|X = x) \left(-\frac{1}{t} - \frac{1}{1-t} \right) + \frac{1}{1-t} \\
 &= \mathbb{P}(Y = 1|X = x) \left(-\frac{1}{t(1-t)} \right) + \frac{1}{1-t} \\
 &= \frac{1}{1-t} \left(1 - \frac{\mathbb{P}(Y = 1|X = x)}{t} \right)
 \end{aligned}$$

For $\mathbb{P}(Y = 1|X = x) \in]0, 1[$, $\mathcal{J}'(t)$ is thus:

- ▶ strictly negative for $t \in]0, \mathbb{P}(Y = 1|X = x)[$,
- ▶ zero at $t = \mathbb{P}(Y = 1|X = x)$,
- ▶ strictly positive for $t \in]\mathbb{P}(Y = 1|X = x), 1[$,

Conclusion: $t = \mathbb{P}(Y = 1|X = x)$ is the unique minimizer on $[0, 1]$ of the function $\mathcal{J}(t)$.

When

- ▶ $\mathbb{P}(Y = 1|X = x) = 0$, $\mathcal{J}(t)$ is minimal at $t = 0$,
- ▶ $\mathbb{P}(Y = 1|X = x) = 1$, $\mathcal{J}(t)$ est minimal at $t = 1$.

We conclude that:

- ① $h^* : x \mapsto \mathbb{P}(Y = 1|X = x)$ is optimal,
- ② $h^*(x)$ is the unique minimizer of the fonction $\mathcal{J} : t \mapsto \mathbb{E}_{Y|X} (L(Y, t)|X = x)$.

In converse : suppose that h optimal.

Let the function:

$$g(x) = \mathbb{E}_{Y/X}(L, Y, h(X))/X = x) - \mathbb{E}_{Y/X}(L, Y, h^*(X))/X = x)$$

We have:

- ▶ $\mathbb{E}_X(g(X)) = \int_{\mathcal{X}} g(x) dP^X = 0$ (otherwise, h would not be optimal),
- ▶ $\forall x, g(x) \geq 0$ by the optimality of h^* .

Therefore, $g = 0$ $P^X - a.e.$, that is:

$$\mathbb{P}(X \in F) = 0 \text{ avec } F = \{x \in \mathcal{X} \text{ t.q. } g(x) > 0\}$$

Solution of exercise 1

[back to questions](#)

$h^*(x)$ is the unique minimizer of the function
 $\mathcal{J} : t \mapsto \mathbb{E}_{Y|X} (L(Y, t) | X = x)$, we have:

$$F = \{x \in \mathcal{X} \text{ t.q. } h(x) \neq h^*(x)\}$$

We conclude that $h = h^* P^X - a.e.$, establishing the desired equivalence.

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Solution of exercise 2

[back to questions](#)

❶ For all $k \in \{1, \dots, K-1\}$:

$$P(Y = k | X = x) = \exp(\beta_k^\top x) P(Y = 0 | X = x).$$

Following $\sum_{k=0}^{K-1} P(Y = k | X = x) = 1$, we have:

$$\begin{cases} P(Y = k | X = x) = \frac{\exp(\beta_k^\top x)}{1 + \sum_{k' \neq 0} \exp(\beta_{k'}^\top x)}, & k \neq 0 \\ P(Y = 0 | X = x) = \frac{1}{1 + \sum_{k' \neq 0} \exp(\beta_{k'}^\top x)} \end{cases} \quad (1)$$

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Solution of exercise 2

[back to questions](#)

② Let $\tilde{k} \neq 0$. Suppose that we select the class \tilde{k} as the reference and for $k \neq \tilde{k}$ the vector $\tilde{\beta}_k$ of the model is given by:

$$\ln \left(\frac{P(Y = k|X = x)}{P(Y = \tilde{k}|X = x)} \right) = \tilde{\beta}_k^\top x, \quad k \neq \tilde{k}$$

Since

$$\begin{aligned} \ln \left(\frac{P(Y=k|X=x)}{P(Y=\tilde{k}|X=x)} \right) &= \ln \left(\frac{P(Y=k|X=x)}{P(Y=0|X=x)} \frac{P(Y=0|X=x)}{P(Y=\tilde{k}|X=x)} \right) \\ &= \beta_k^\top x - \beta_{\tilde{k}}^\top x, \end{aligned}$$

we have:

$$\begin{cases} \tilde{\beta}_k &= \beta_k - \beta_{\tilde{k}}, \quad k \neq 0, \quad k \neq \tilde{k} \\ \tilde{\beta}_0 &= -\beta_{\tilde{k}} \end{cases} \quad (2)$$

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Solution of exercise 2

[back to questions](#)

By using the results of Question ①, we have that for $k \neq \tilde{k}$:

$$\begin{cases} P(Y = k|X = x) &= \frac{\exp(\tilde{\beta}_k^\top x)}{1 + \sum_{k' \neq \tilde{k}} \exp(\tilde{\beta}_{k'}^\top x)}, \quad k \neq \tilde{k} \\ P(Y = 0|X = x) &= \frac{1}{1 + \sum_{k' \neq \tilde{k}} \exp(\tilde{\beta}_{k'}^\top x)} \end{cases}$$

By substituting $\tilde{\beta}_k$ in these equations using the relations (2), we obtain the equations (1).

Summary: Changing the reference class alters the model's parameters (without changing the model itself).

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③ To establish the connection with binary logistic regression, we represent the observation $y_i \in \{0, \dots, K-1\}$ by the vector $z_i \in \{0, 1\}^K$:

$$z_{i,k} = \begin{cases} 1 & \text{if } y_i = k \\ 0 & \text{otherwise} \end{cases}$$

We also denote β the set of vectors $\beta_1, \dots, \beta_{K-1}$.

We express the likelihood associated with the example (x_i, y_i) :

$$\begin{aligned} P_{\beta}^{Y_i|X_i}(y_i|x_i) &= \prod_{k=0}^{K-1} P_{\beta}^{Y_i|X_i}(k|x_i)^{z_{i,k}} \\ &= P_{\beta}^{Y_i|X_i}(0|x_i)^{1-z_{i,1}-\dots-z_{i,K-1}} \left(\prod_{k=1}^{K-1} P_{\beta}^{Y_i|X_i}(k|x_i)^{z_{i,k}} \right) \\ &= P_{\beta}^{Y_i|X_i}(0|x_i) \prod_{k=1}^{K-1} \left(\frac{P_{\beta}^{Y_i|X_i}(k|x_i)}{P_{\beta}^{Y_i|X_i}(0|x_i)} \right)^{z_{i,k}} \end{aligned}$$

Using :

- ▶ the $(K - 1)$ regression models:

$$\frac{P_{\beta}^{Y_i|X_i}(k|x_i)}{P_{\beta}^{Y_i|X_i}(0|x_i)} = \exp(\beta_k^{\top} x_i)^{z_{i,k}},$$

- ▶ the second equation of (1):

$$P(Y = 0|X = x) = \frac{1}{1 + \sum_{k'=1}^{K-1} \exp(\beta_{k'}^{\top} x)},$$

the log-likelihood is expressed as:

$$\ell(\beta) = \sum_{k=1}^{K-1} \sum_{i=1}^n z_{i,k} \beta_k^{\top} x_i - \ln \left(1 + \sum_{k'=1}^{K-1} \exp(\beta_{k'}^{\top} x_i) \right)$$

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Generalized linear models

Definition

The GLM contains all statistical models such that

- ▶ $Y|X$ follows a distribution from an **exponential family**:

$$f^{Y|X}(y|x) = C(\eta)h(y)\exp(\eta y) \quad \text{with } \eta = \eta(x).$$

- ▶ $g(\mathbb{E}_\beta(Y|X = x)) = \beta_0 + \beta^\top x$.

Vocabulary. The function g is called the **link function**.[†]

Example. Bernoulli distributions form an exponential family.

$$\begin{aligned} f(y) &= \theta^y (1 - \theta)^{1-y} \\ &= (1 - \theta) \exp\left(\ln\left(\frac{\theta}{1 - \theta}\right)y\right) \quad \Rightarrow \eta = \ln\left(\frac{\theta}{1 - \theta}\right) \end{aligned}$$

[†] Let N denote the set of admissible value for η : g is often chosen to be a bijection from N to \mathbb{R} .

Remark: generalized linear models (GLM)

The logistic regression model has the form

- ▶ $Y|X \sim \text{Ber}(\mathbb{E}_\beta(Y|X))$,
- ▶ $g(\mathbb{E}_\beta(Y|X)) = \beta_0 + \beta^\top X$, with $g = \text{logit}$.

⇒ special case of the **generalized linear model (GLM)**
(g is called link function)

⇒ complement

Remark: we have already met another GLM model

- ▶ $Y|X \sim \mathcal{N}(\mathbb{E}_\beta(Y|X), \sigma^2)$
- ▶ $g(\mathbb{E}_\beta(Y|X)) = \beta_0 + \beta^\top X$ with $g = \text{Id}$

Example: $Y_i|X_i \stackrel{\text{iid}}{\sim} \text{Poisson}(\theta_i)$, with $\ln \theta_i = \beta_0 + \beta_1 X_i$

Poisson distributions form an exponential family:

$$\begin{aligned} f(y) &= \exp(-\theta) \frac{\theta^y}{y!} \\ &= \frac{1}{y!} \exp(-\theta) \exp(\ln(\theta)y) \quad \Rightarrow \eta = \ln(\theta) \end{aligned}$$

