

# Machine Learning - Week 2

Maestría en Ciencia con mención de Tecnología de la información

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## Presentación

- 2021 Nov. Machine Learning Ops., Warner Bros. Entertainment, France.
- 2020 2021 Research And Teaching Assistant, Université de Technologie de Compiègne (UTC), France.
- 2018 2020 PhD in Computer Science, University of Technology of Compiègne, Compiègne France. Distributionally robust, skeptical inferences in supervised classification using imprecise probabilities
- 2015 2017 M.S in Applied Mathematics, University of Montpellier, France. Majoring in Biostatistics, Health-Economic modeling using Markov model and application in R
- 2013 2015 M.S in Computer Science, University of Montpellier, France. Majoring in Data, Knowledge and Natural Language, Modelling of the users behaviour for Crowdsourcing platform to large scale



- 2011 2012 Diploma Course in Project Management, Institute San Ignacio de Loyola, Lima, Pérou. Project Management based on the focus of the Project Management Institute PMI
- 2004 2009 Bachelor in Computer Science, National University of San Marcos, Lima, Peru. Computers and Systems
- 2007 2012 Senior Developer Analyst, Lima Peru.

# **Overview**

Supervised learning Supervised classification Problem setting Classical classification methods Example of classification in python Linear regression Problem setting Classical methods Example of regression in Python NLP and Other advanced supervised methods Multi-label and Label ranking Image patter recognition Natural Language Processing **Bias-variance tradeoff** Interpretability and explainability of ML methods

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# **Overview**

#### Supervised learning

Supervised classification

Problem setting

**Classical classification methods** 

Example of classification in python

Linear regression

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**Classical methods** 

Example of regression in Python

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Multi-label and Label ranking

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# Outline of supervised learning problem.

#### Historical data (training data)



Figure: Learn a recruitment and selection process model.

# Supervised learning

Any learning process is based on knowledge acquisition, be it implicit, explicit, or both. *That is how it happens in humans and not too differently in computers*.

Computers focuses on a *specific and particular task*, in which it learns to generalize repetitive and similar patterns of a well-framed and well-specific experiment, e.g. classification of images.

#### Objective

Learn a *model* that minimizes the risk of making a wrong decision.

## Mathematical formulation

Let  $\mathscr{D} = \{(\mathbf{x}_i, y_i) | i = 1, ..., N\} \subseteq \mathscr{X}^p \times \mathcal{K}$  be a training data set generated from an unknown joint probability distribution  $\mathbb{P}$ 

- A response variable *Y* (also called output, target, outcome)
- A vector of *p* predictors *x* (also called inputs, features, attributes, explanatory variables)

The goal is to build a predictive model  $\varphi: \mathscr{X} \to \mathscr{K}$  that minimizes the risk of making a wrong decision by computing

$$\mathcal{R}(\varphi) = \mathbb{E}_{X \times Y} \left[ \ell(Y, \varphi) \right] = \int_{\mathscr{X} \times \mathscr{K}} \ell(y, \varphi(\mathbf{x})) d\mathbb{P}(\mathbf{x}, y), \tag{1}$$

expected value of a specified loss  $\ell(\cdot, \cdot)$  :  $\mathscr{K} \times \mathscr{K} \to \mathbb{R}$  penalizing every wrong decision.

**X** Equation (1) is however impossible to compute since  $\mathbb{P}$  is unknown !!

## Mathematical formulation

Let  $\mathscr{D} = \{(\mathbf{x}_i, y_i) | i = 1, ..., N\} \subseteq \mathscr{X}^p \times \mathcal{K}$  be a training data set generated from an unknown joint probability distribution  $\mathbb{P}$ 

- A response variable *Y* (also called output, target, outcome)
- A vector of p predictors x (also called inputs, features, attributes, explanatory variables)

In practice we use the empirical risk minimization (ERM) principle as follows

$$\mathscr{R}(\varphi) = \frac{1}{N} \sum_{i=1}^{N} \ell(y_i, \varphi(x_i)).$$
(1)

Note that if we have too much of training observations:  $\mathscr{R}(\varphi) \xrightarrow[N \to \infty]{} \mathcal{R}(\varphi)$ 

#### Objective

Learn an  $\varphi$  "optimal" model that minimizes Equation (1).



## **Recommended readings**

- "An Introduction to Statistical Learning" (ISLR): emphasis on basic principles and application, no mathematical details. Available at https://www.statlearning.com/.
- "The Elements of Statistical Learning" (ESL): more mathematically advanced and theoretical. Available at http://statweb.stanfor edu/~tibs/ElemStatLearn



# **Overview**

Supervised learning

#### Supervised classification

# **Binary classification**

#### Example

Let us consider a binary classification problem, in which we need identify if the new observation is a Dog or a Cat.



Figure: Dogs and Cats

# **Binary classification**

#### Example

Let us consider a binary classification problem, in which we need identify if the new observation is a Dog or a Cat.



Figure: Dogs and Cats

Figure: New observation

What class does the new observation belongs to?

It is the one that has the highest probability (or score).

# **Binary classification**

#### Example

Let us consider a binary classification problem, in which we need identify if the new observation is a Dog or a Cat.



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## **Outline of classification problem**

Given the training data  $\mathscr{D} = \{x_i, y_i\}_{i=0}^N \subseteq \mathbb{R}^p \times \{m_a, \dots, m_e\}$ : Step **1** Learning a classification rule:  $\varphi : \mathcal{X} \to \mathcal{K}$ . Step **2** Making decision on a new instance  $\widehat{\varphi}(\mathbf{x}), \mathbf{x} \in \mathscr{T}$ 



Figure: Supervised learning in a precise approach.

## Mathematical formulation - Classification

Let  $\mathscr{D} = \{(\mathbf{x}_i, y_i) | i = 1, ..., N\} \subseteq \mathscr{X}^p \times \mathcal{K}$  be a training dataset  $\mathcal{R}(\varphi) = \arg\min_{\varphi \in \mathcal{K}} \mathbb{E}_{X \times Y} [\ell(Y, \varphi))]$ 

Under 1/0 loss function  $\ell_{0/1}$ , minimizing  ${\cal R}$  is equivalent to

$$\phi(\mathbf{x}^*|\mathscr{D}) := \underset{m_k \in \mathcal{K}}{\arg \max} P(Y = m_k | X = \mathbf{x}^*), \tag{3}$$

where the last equation; (1) is also known as Bayes classifier and (2) predicts the class  $\hat{y}^* = \phi(\mathbf{x}|\mathscr{D})$  the most probable.

(2)

# **Mathematical formulation - Classification**

Let  $\mathscr{D} = \{(\mathbf{x}_i, y_i) | i = 1, ..., N\} \subseteq \mathscr{X}^p \times \mathcal{K}$  be a training dataset  $\mathcal{R}(\varphi) = \underset{\varphi \in \mathcal{K}}{\arg \min} \mathbb{E}_{X \times Y}[\ell(Y, \varphi))]$  (2)

Under 1/0 loss function  $\ell_{0/1},$  minimizing  ${\cal R}$  is equivalent to

$$\phi(\mathbf{x}^*|\mathscr{D}) := \underset{m_k \in \mathcal{K}}{\arg \max} \, \frac{P(Y = m_k | X = \mathbf{x}^*)}{m_k \in \mathcal{K}}, \tag{3}$$

where the last equation; (1) is also known as Bayes classifier and (2) predicts the class  $\hat{y}^* = \phi(\mathbf{x}|\mathscr{D})$  the most probable.

#### In practice

**Step 1** Learning the conditional probability distribution  $\mathbb{P}_{Y|x}$ .

**Step 2** Predicting the "optimal" label amongst  $\mathcal{K} = \{ m_1, ..., m_K \}$ :

$$m_{i_{K}} \succ m_{i_{K-1}} \succ \ldots \succ m_{i_{1}} \iff P(y = m_{i_{K}} | \boldsymbol{x}) > \ldots > P(Y = m_{i_{1}} | \boldsymbol{x})$$

Reference Pick out the most preferable label  $m_{i_K}$ 

 $\iff$  maximal probability plausible  $P(y = m_{i_k} | \mathbf{x})$ 

## Gaussian Discriminant Analysis

**Assumptions:** Conditional probability  $P_{X|Y=m_k} \sim \mathcal{N}(\mu_k, \Sigma_{m_k}), \forall m_k$ **Learning**  $\mathbb{P}$ : Maximum likelihood estimation or Bayesian inference.

Discriminant analysis model	Assumptions ( $\forall m_k \in \mathcal{K}$ )	Parametric space ( $orall m_k \in \mathcal{K}$ )
Parametric Gaussian conditional distribution $\mathbb{P}_{X Y=m_k}$		
Linear Discriminant [3, §4.3]	Homoscedasticity: $\Sigma_{m_k} = \Sigma$	$\Theta = \{\theta_{m_k}   \theta_{m_k} = (\pi_{m_k}, \Sigma, \mu_{m_k})\}$
Quadratic Discriminant [3, §4.3]	Heteroscedasticity: $\Sigma_{m_k} = \Sigma_k$	$\Theta = \{\theta_{m_k}   \theta_{m_k} = (\pi_{m_k}, \Sigma_k, \mu_{m_k})\}$
Naive Discriminant [3, §6.63]	Feature independence: $\Sigma_{m_k} = \boldsymbol{\sigma}_k^T \mathbb{I}$	$\Theta = \{\theta_{m_k}   \theta_{m_k} = (\pi_{m_k}, \sigma_k, \mu_{m_k})\}$
Euclidean Discriminant [6]	Unit-variance feature indep.: $\Sigma_{m_k} = \mathbb{I}$	$\Theta = \{ heta_{ extsf{m}_k}    heta_{ extsf{m}_k} = (\pi_{ extsf{m}_k}, \mu_{ extsf{m}_k})\}$

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# **Classical classification methods**

## Gaussian Discriminant Analysis

**Assumptions:** Conditional probability  $P_{X|Y=m_k} \sim \mathcal{N}(\mu_k, \Sigma_{m_k}), \forall m_k$ **Learning**  $\mathbb{P}$ : Maximum likelihood estimation or Bayesian inference.





**QDA** 



Figure: Gaussian discriminant models

## Logistic regression

#### **Assumptions:**

If  $Y = \{0, 1\}$  (binary classification) so  $\mathbb{P}_{Y=1|x,\beta} \sim \mathcal{B}er(\psi(\beta^T x))$ , where

$$P(Y=1|X=x,\beta) := \psi(\beta^T x) = \frac{e^{\beta^T x}}{1+e^{\beta^T x}}$$

In case of multi-class classification,  $\mathbb{P}_{Y|x,beta} \sim Cat(\beta_{m_1}, \dots, \beta_{m_k})$ .

$$P(Y = m_k | X = x, \beta_{m_k}) := rac{e^{eta_{m_k}^T X}}{\sum_{l=1}^K e^{eta_{m_l}^T X}}$$

**Learning**  $\mathbb{P}$ : Maximum likelihood estimation or Bayesian inference (but both using approximative methods to get optimal value of parameter  $\beta_*$ 

# **Classical classification methods** (Multi-class) Multinomial Logistic regression

Decision surface of LogisticRegression (multinomial)

Why it is linear?

→ All points in the boundary must satisfy:  $\{x : \psi(\beta_0^T x) = \psi(\beta_1^T x)\}$ 

$$(\beta_0^T - \beta_1^T)x = 0$$

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#### K-nearest neighbors algorithm

Let  $\mathscr{D} = \{(\mathbf{x}_i, \mathbf{y}_i) | i = 1, ..., N\}$  dataset and a neighbourhood  $N_k(\cdot)$  of K neighbors.

$$\psi(\mathbf{x}) = \arg \max_{\mathbf{y} \in \mathscr{K}} \frac{1}{K} \sum_{\mathbf{x}_i \in N_K(\mathbf{x})} \mathbb{I}_{\mathbf{y} = = \mathbf{y}_i}$$



K-nearest neighbors algorithm

Let  $\mathscr{D} = \{(\mathbf{x}_i, \mathbf{y}_i) | i = 1, ..., N\}$  dataset and a neighbourhood  $N_k(\cdot)$  of K neighbors.

$$\psi(\mathbf{x}) = \arg \max_{\mathbf{y} \in \mathscr{K}} \frac{1}{K} \sum_{x_i \in N_K(\mathbf{x})} \mathbb{I}_{\mathbf{y} = = \mathbf{y}_i}$$



K-nearest neighbors algorithm

Let  $\mathscr{D} = \{(\mathbf{x}_i, y_i) | i = 1, ..., N\}$  dataset and a neighbourhood  $N_k(\cdot)$  of K neighbors.

$$\psi(x) = \arg \max_{y \in \mathscr{K}} \frac{1}{K} \sum_{x_i \in N_K(x)} \mathbb{I}_{y = = y_i}$$







#### Tree-based models (Random Forest, Bagging, ...)

Prediction the salary in millions = Y



#### Tree-based models (Random Forest, Bagging, ...)



#### Tree-based models (Random Forest, Bagging, ...)



#### Tree-based models (Random Forest, Bagging, ...)



#### Tree-based models (Random Forest, Bagging, ...)







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#### Tree-based models (Random Forest, Bagging, ...)



#### Tree-based models (Random Forest, Bagging, ...)



#### Tree-based models (Random Forest, Bagging, ...)

X Tree-based models are not always good !!



## Tree-based models (Random Forest, Bagging, ...)

#### ✓ Bagging or Random Forest method



- Weighted prediction
- Non-linear decision boundaries



# **Classical classification methods** Support Vector Machine - Classification

The margin of H is the smallest distance between H and a vector  $x_i$ 

$$M = \arg\min_{i} d(x_i, H) = \arg\min_{i} \frac{\beta^T (x - x_0)}{||\beta||}$$
(4)



#### **Support Vector Machine - Classification**

The Optimal Separating Hyperplane is the hyperplane with the largest margin. It can be found by solving the optimization problem:

$$M \iff \arg\min_{\beta} \frac{1}{2} ||\beta||^2$$
 (4)

subject to 
$$y_i(\beta^T x_i + \beta_0) \ge 1 - \xi_i, i = 1, ..., n$$
 (5)



## **Support Vector Machine - Classification**

The Optimal Separating Hyperplane is the hyperplane with the largest margin. It can be found by solving the optimization problem:

$$M \iff \arg\min_{\beta} \frac{1}{2} ||\beta||^2$$
 (4)

subject to  $y_i(\beta^T x_i + \beta_0) \ge 1 - \xi_i, i = 1, ..., n$  (5)



Others: XGBoost, Neural Network, Deep-Learning....



## Others: XGBoost, Neural Network, Deep-Learning....



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## Others: XGBoost, Neural Network, Deep-Learning....

XGBoost





#### **Deep-Convolution neural network**



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#### **Example of classification**

# Let us do Machine Learning Code source - [Link]

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## Mathematical formulation - Regression

Let  $\mathscr{D} = \{(\mathbf{x}_i, y_i) | i = 1, \dots, N\} \subseteq \mathscr{X}^p \times \mathcal{K}$  be a training dataset

$$\mathcal{R}(\varphi) = \underset{\varphi \in \mathcal{F}}{\arg\min} \mathbb{E}_{X \times Y} \left[ \ell(Y, \varphi) \right]$$
(6)

Under squared loss function, minimizing  $\mathcal{R}$  is equivalent to

$$\varphi(\cdot) := \underset{\varphi \in \mathcal{F}}{\arg\min} \int_{\mathscr{X} \times \mathscr{Y}} (y - \varphi(\mathbf{x}))^2 \mathrm{d}\mathbb{P}(\mathbf{x}, y), \tag{7}$$
$$\varphi(\mathbf{x}^*) := \mathbb{E}(Y | X = \mathbf{x}^*), \tag{8}$$

where the last equation amounts to saying that

- Prediction may be interpreted as an average value.
- Again the conditional distribution  $\mathbb{P}_{Y|X}$  is unknown.

#### K-nearest neighbors algorithm

Let  $\mathscr{D} = \{(\mathbf{x}_i, \mathbf{y}_i) | i = 1, ..., N\}$  dataset and a neighbourhood  $N_k(\cdot)$  of K neighbors.

$$arphi(x) = \mathsf{Ave}\left\{y_i : x_i \in \mathsf{N}_{\mathsf{K}}(x)
ight\} = rac{1}{\mathsf{K}}\sum_{x_i \in \mathsf{N}_{\mathsf{K}}(x)} y_i$$



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#### Linear regression

**Assumptions:** Expectation value can be written as a linear equation  $\beta^T x$ .

$$\varphi(\mathbf{x}_{i}^{*}) := Y_{i} := \underbrace{\beta^{0} + \sum_{j=1}^{p} \beta^{j} \mathbf{x}_{i}^{j}}_{\mathbb{E}(Y|X=\mathbf{x}^{*})} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^{2})$$
(9)



Let  $\mathscr{D} = \{(\mathbf{x}_i, y_i) | i = 1, ..., N\}$  a dataset. The most popular estimation method for  $\beta$  parameters is **least squares**, in which we minimize the sum of squared residuals (differences between  $y_i$  and  $\varphi(\mathbf{x}_i^*)$ ). And where the optimal values of  $\beta$  is

$$\beta = (X^T X)^{-1} X^T y$$

#### **Linear regression**

**Assumptions:** Expectation value can be written as a linear equation  $\beta^T x$ .

$$\varphi(\mathbf{x}_{i}^{*}) := Y_{i} := \beta^{0} + \sum_{j=1}^{p} \beta^{j} x_{j}^{j} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^{2})$$
(9)  
Reported happiness as a function of income  

$$\varphi(\mathbf{x}_{i}^{*}) := Y_{i} := \beta^{0} + \sum_{j=1}^{p} \beta^{j} x_{j}^{j} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^{2})$$
(9)

Income (x\$10,000)

# Classical regression methods Regularized Linear regression

In order to avoid the overfitting and other issues, an regularized component is added:

$$\mathcal{R}^{*}(\varphi(x)) = \underset{\varphi \in \mathcal{F}}{\arg\min} \mathbb{E}\left[ (Y - \varphi(x))^{2} \middle| X = x \right] + \Upsilon(\varphi)$$
(10)

- Ridge regression
- Lasso regression
- Elastic net
- Principal component regression
- Partial least squares regression

#### Other regression methods

The base classification models used previously can also be adapted to the regression problem:

- 1. Tree-based model
- 2. Random Forest, Bagging, Boosting, ...
- 3. Support Vector Machine for regression
- 4. XGboost for regression
- 5. Deep-learning models

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## **Example of regression**

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# Multi-label classification problem

The goal of multi-label problem:

Given a training data:  $\mathscr{D} = \{ \mathbf{x}^i, \mathbf{y}^i \}_{i=0}^N \subseteq \mathbb{R}^p \times \mathscr{Y}$ 

where:  $\mathscr{Y} = \{0,1\}^m, \quad |\mathscr{Y}| = 2^m$ 

Learning a multi-label classification rule:  $\varphi : \mathbb{R}^p \to \mathscr{Y}$ 



## Label-wise ranking problem

#### reason The goal of label ranking problem:

Given a training data:  $\mathscr{D} = \{\mathbf{x}_i, Y_i\}_{i=0}^N \subseteq \mathbb{R}^p \times \Lambda(\mathscr{K})$ Learning a complete ranking rule:  $\varphi : \mathbb{R}^p \to \Lambda(\mathscr{K})$ 



#### Figure: Label-wise decomposition

# Handwritten ZIP code.

**Problem:** Identify the numbers in a handwritten ZIP code, from a digitized image



The task is to recognize, from the matrix of pixel intensities, the digit in each image (0, 1, ..., 9) quickly and accurately. We can use any base classifier model

- Support Vector Machine
- Deep-learning models
- Others (logistic, ...)

# **Recognize the expression on a face.**

**Problem:** Identify the expression on a face.





surprise



sadness



disgust









fear

#### Figure: Expression recognition

## How can we solve these problems?

A simple approach may be:

- 1. to save all pixel values of images in a record, in which their values is ranging in intensity from 0 to 255.
- 2. to use an unsupervised method to reduce the dimensionality of *X* input space, and then, to apply a base classifier method.



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#### Natural Language Processing



## Natural Language Processing



Very intuitive platform, I'll definitely recommend it. The chat support is excellent, really fast in their replies and very helpful.

Usability

Positive

Customer Support

- 1. How can we work with unstructured data?
- 2. Are there mathematics tools?

#### **Representation as vector** $\mathbb{R}$



## **Representation as vector** $\mathbb{R}$ - **BagWords**



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## Representation as vector $\mathbb R$ - Term frequency



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## Representation as vector ${\ensuremath{\mathbb R}}$ - One-hot encoded



#### **Representation as vector** $\mathbb{R}$

#### Given three english texts



Word embedding is another powerful way to work with text.In an euclidian space, we can use any base classifier model.

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## **Bias-variance tradeoff**

How accurate can we be predicting?



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## Interpretability/flexibility trade-off



#### Explainability ML using SHapley Additive exPlanations



i went and saw this movie last night after being coaxed to by a few friends of mine . i ' II admit that i was reluctant to see it because from what i knew of ashton kutcher he was only able to do comedy. i was wrong. kutcher played the character of jake fischer very well, and kevin costner played ben randall with such professionalism. the sign of a good movie is that t can toy with our emotions, this one did exactly that the entire theater ( which was sold out ) was overcome by laughter during the



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Thank You for Your Attention!