Ensemble learning from theory to practice

Lecture 1:
Part 1: Introduction - Part 2: Decision Trees

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CentraleSupélec

About me

- Undergrad at the Univ. of Montpellier (UM), France
- Ph.D. in IMAG lab at UM, France
- Postdoc researcher in LIG lab at Univ. of Grenoble Alpes, France
- Associate Professor Maître de ConFérences (MCF) at CentraleSupélec & MICS lab since 2019 (HDR in 2025)
- Co-responsible MSc in AI
- Coordinator of many research project fundings (ANR JCJC, etc.)
- Member of many scientific associations and scientific commitees

Research interests: ML, Ensemble methods, Few-supervised ML methods, Domain adaptation, Heterogeneous data, Multi-modal learning, Causality.

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Course organization

- **9 class hours**
- **12 practical class hours** (practical exercises, labs using Python, 3 hours for the Python project)
- **3 hours for each group oral defense** of an evaluated Python project (date to define)
- Main instructor:
  - Myriam Tami
  - Office hours: send me an email and we will find a good time to meet
  - **Best way to get a quick answer: by email (answering delay: 3-7 days)**
- **Evaluation**: project using python (with code $\rightarrow$ GIT and oral defense $\rightarrow$ slides), individual assignments.

Teaching tools

- **Edunao**:
  - More details about the course and the organization (timeline, etc.)
  - Teaching material (slides, Jupyter Notebooks, PDF with practical exercices, corrections.)
  - Resources (books, papers)
  - Submit your work
- **Microsoft Teams**:
  - If you are sick, please let me know, and we will use Teams

Coursework and grading (subject to change)

	Wght	Details
Assignment (individual)	25%	Theoretical questions or exercises
Python project (teams of 2 students)	75%	**Project proposal** (to send by email before the next session; code (GIT link) and slides to submit on edunao before (to define); **oral defense in class planed for the last session**

Previous project (2020)

Text Classification with Rakuten France Product Data

- Topic of large-scale product type code text classification
- This project is derived from a data challenge (details available in this link)
- Goal: predict each product's type code as defined in the catalog of Rakuten France
- The above data challenge focuses on multimodal product type code classification using text and image data

Previous project (2020)

Tasks for the Rakuten project:

- After a preprocessing step, build a TF-IDF matrix that will constitute the data set
- The project guidelines was:
  - Apply all adapted approaches of the course and handled during labs (Decision Trees, Bagging, Random forests, Boosting, Gradient Boosted Trees, AdaBoost, etc.) on this data set in the goal to predict the target variable (product's type code).
  - Compare their performances thanks all scores you can output.
  - Conclude about the most appropriate approach on this data set for the predictive task.
  - Write a report in .tex format that adress all these guidelines. We will take into account the quality of writing and presentation of the report.
  - **Provide a GIT link of your team Python code and allow to show your work progress.**

Others previous projects (2022, 2023)

- 2022: Cyberbullying Classification (cf. template on Edunao)
- 2023: Predicting Airbnb Prices in New York City (cf. template on Edunao)
- 2024: Predicting daily Electricity Price variation and Explaination (in France and Germany)

Project of this year

I propose to you to submit the project subject you are interested to work on it!

The guidelines:

- Take inspiration from the previous project or any datachallenge from the web (e.g., Challenge data - ENS, etc.)
- Try to propose a project i.e.: an ML task on a reasonable dataset: a huge dataset could be too hard to work on it (too time consuming)
- The project guidelines stay the same (apply all appropriate approaches of the course, compare and present the results and performances, conclude, provide slides, provide the GIT link of your code...)

Prerequisites in ML

Given an ML problem,

- Decide as what type of ML problem you can formalize it:
  - Supervised? Unsupervised?
  - Regression? Classification? Clustering?
  - Dimensionality reduction?
- Describe it formaly in terms of
  - A design matrix X (n, d) dim
  - A target variable/matrix Y
  - A loss function to optimize
- Apply the ML pipeline (data preprocessing, model selection, evaluation, make prediction; etc.)
- Programming (Python, scikit-learn, numpy, pandas, scipy, etc)
- Deal with real-world data challenges

Prerequisites in Decision Trees (DT)

DT (based classification) building

- A simple, greedy, recursive approach (builds up tree node-by-node)
  - Split a set of data points based on an attribute test condition that optimizes a specific criterion
  - How to determine the best split (i.e., the best attribute test condition and the best split value)
  - Stopping criteria for DT growing and overfitting problem
- Know some measures of node impurity (e.g., Gini index)
- Read a DT visualization (diagram)

Learning objectives of the course

Given an ML problem,

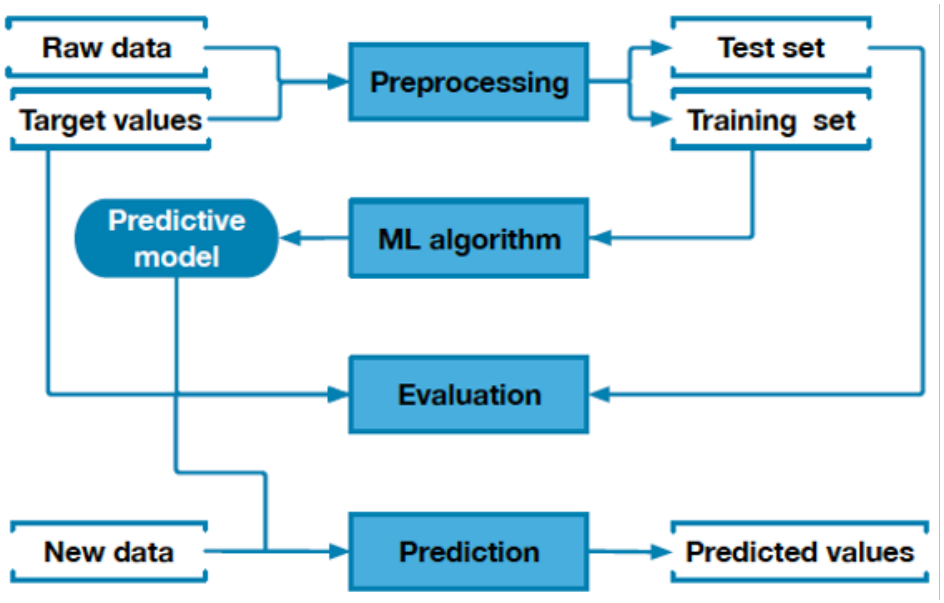
- Know if you can use an ensemble method to solve it
- Know as what type of ensemble methods can correspond it
- Can formalize it by using a model from ensemble methods models
- Can apply/learn/tune different models from ensemble methods
- For each of them, can make an evaluation and comparison to choose the more appropriate model
- Know the pros and cons of each ensemble method or tree-based approach
- Understand and know the theoretical process/algorithms of each ensemble method
- Can implement each of them from scratch (option a.) or by using Python libraries
- Be able to read, understand and restitute the content of a research paper (option b.)

Learning objectives of the today's class

- Reminders (ML, DT) and introduce our ML notations, formalizations
- Present DT building process:
  - mathematical rules for regression AND classification cases
  - the algorithms
- Be able to formalize and understand in details the DT building process
- Know more about the DT limitations
- Be able to implement DT algorithms by yourself (by using scikit-learn library or from scratch):
  - know how to train and visualize a DT
  - learn how to predict with a DT and how to regularize it
  - know how to use DT for regression/classification tasks

Traditional ML process,

- You have a data set (both input and target)
- You have to achieve a task (i.e., classification, regression)
- To tackle it: you learn a predictor (a predictive model)!



But, **What happen if you obtain a weak learner?**
meaning it does only slightly better than random guessing

Together we stand but divided we fall!

- Ensemble learning principle: **combine multiple weak learners in order to improve robustness and prediction performances**

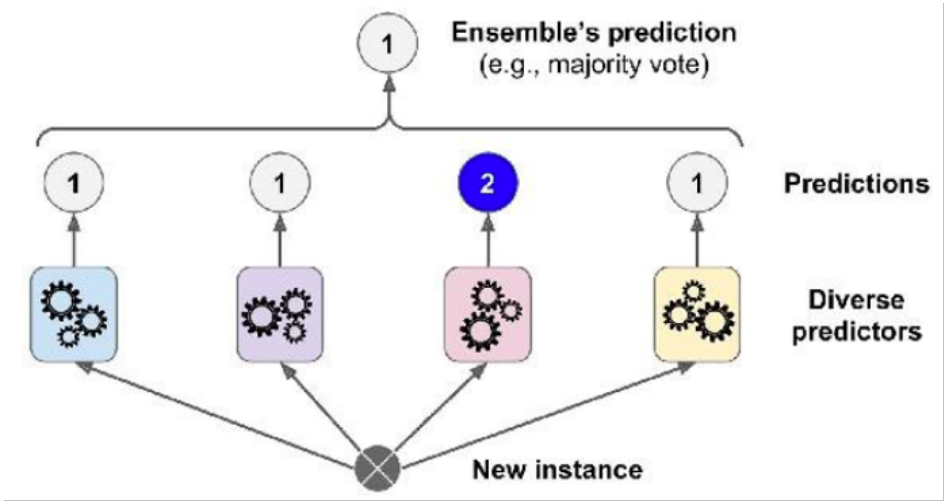


Figure: source: Hands-On Machine Learning with Scikit-Learn and TensorFlow, A. Géron

- A decision tree is a weak learner
- Intuition: an aggregation of weak Decision Trees (DT) leads to a strong random forest

Before, we have to come back to DT in details

Introduction and history

- Decision tree method was introduced by Leo Breiman in 1984
- There are many algorithms:
  - CART (Classification And Regression Trees) [Breiman et al., 1984]
  - ID3, C4.5
  - Hunt
- Python library: `scikit-learn` (`sklearn` module)

Introduction and notations

- A decision tree is a weak **supervised** learner
- **Goal**: predict a dependent variable $y \in \mathcal{Y}$ explained by input variables $x \in \mathcal{X}$ via a set of data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ iid

Related goals:

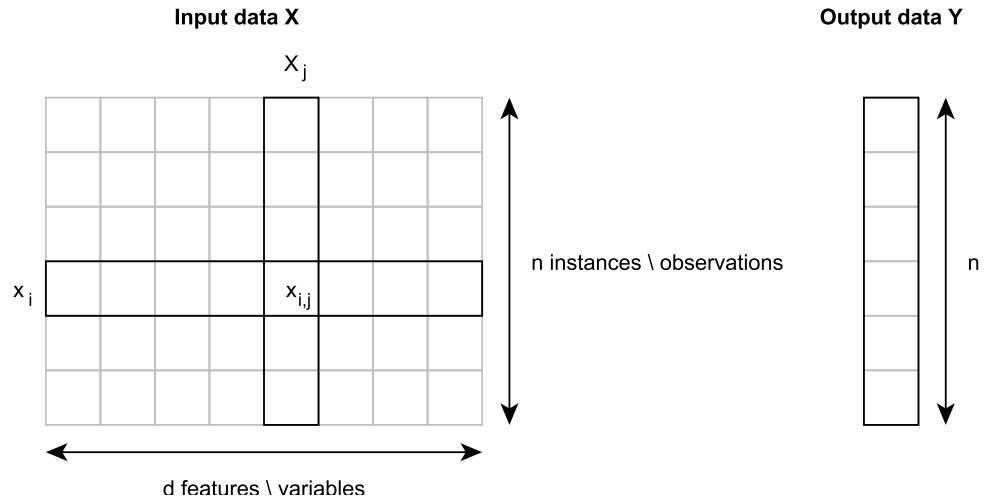
Construct a predictor $\hat{f}(x)$ of a function f mapping x to y

$$f : \mathcal{X} \to \mathcal{Y}$$
$$x \mapsto y$$

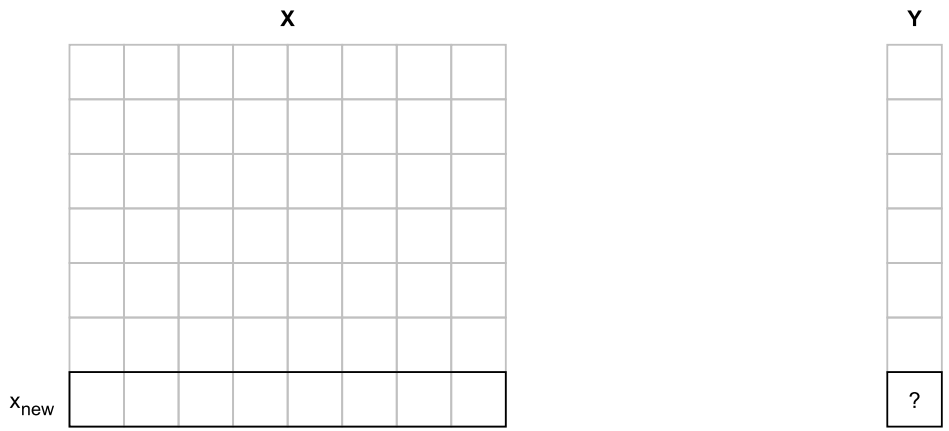
- for supervised **regression**: $\mathcal{Y} = \mathbb{R}$ and $\mathcal{X} = \mathbb{R}^d$
- for supervised **classification**: $\mathcal{Y} = \{1, \ldots, C\}$ and $\mathcal{X} = \mathbb{R}^d$ where C is the number of classes and d the dimension of the input space $\mathcal{X}$

Supervised learning problematic

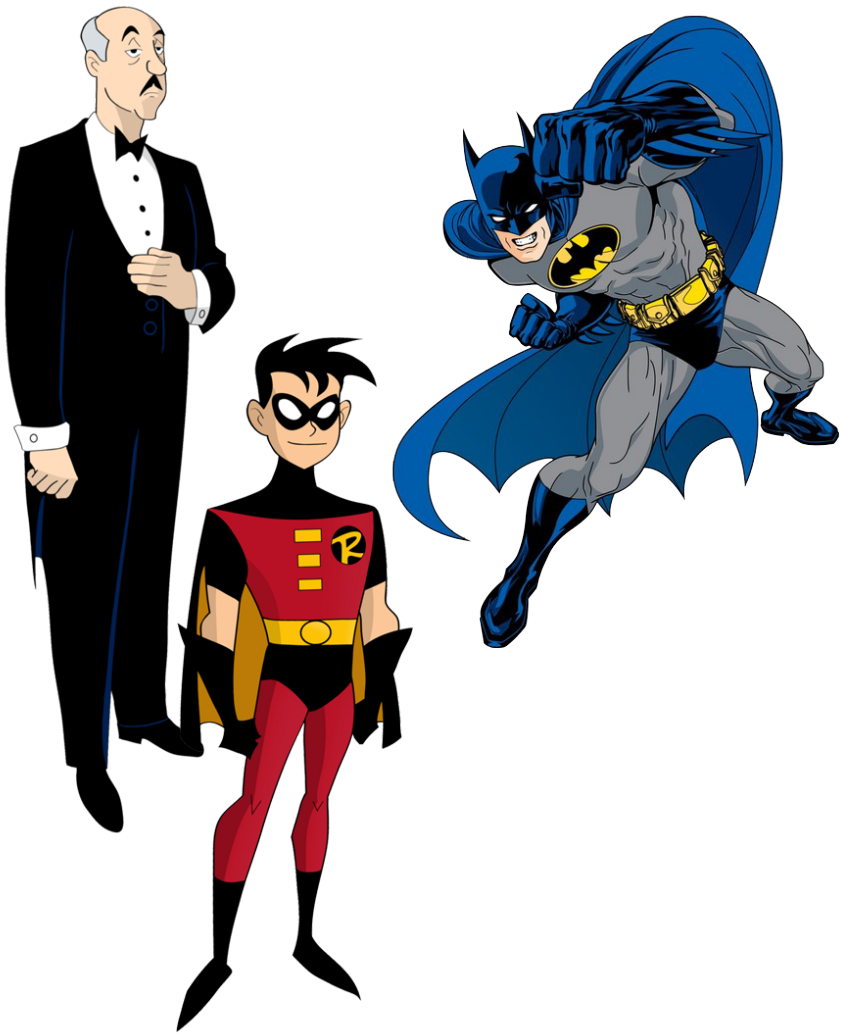
- The data



- Related problematic:
  For a new observation x_{new} I want to predict the linked unobserved y



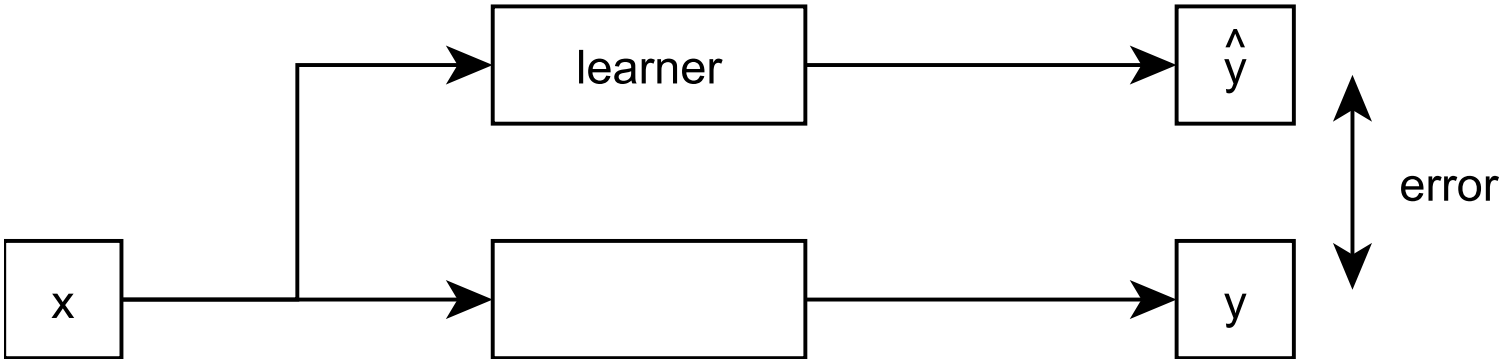
Example of supervised learning problematic



Problem: Is your date good or evil?

	mask	cape	tie	ears	smokes	height	class
Batman	y	y	n	y	n	180	**good**
Robin	y	y	n	n	n	176	**good**
Alfred	n	n	y	n	n	185	**good**
Penguin	n	n	y	n	y	140	**evil**
Catwoman	y	n	n	y	n	170	**evil**
Joker	n	n	n	n	n	179	**evil**
Batgirl	y	y	n	y	n	165	**?**
Riddler	y	n	n	n	n	182	**?**
Someone New	n	y	y	y	y	181	**?**

Supervised learning



1. Set of couples (x_i, y_i), $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ learning set
2. $x_i \in \mathcal{X}$ e.g., $\mathcal{X} = \mathbb{R}^d$ and x_i a d-length vector
   $y_i \in \mathcal{Y}$ e.g., $\mathcal{Y} = \mathbb{R}$ if y a temperature feature or $\mathcal{Y} = \{0, 1\}$ if y encodes the class evil v.s good
3. The learner select among a given set of functions $\mathcal{F}$, the best f such as $\hat{y} = f(x)$

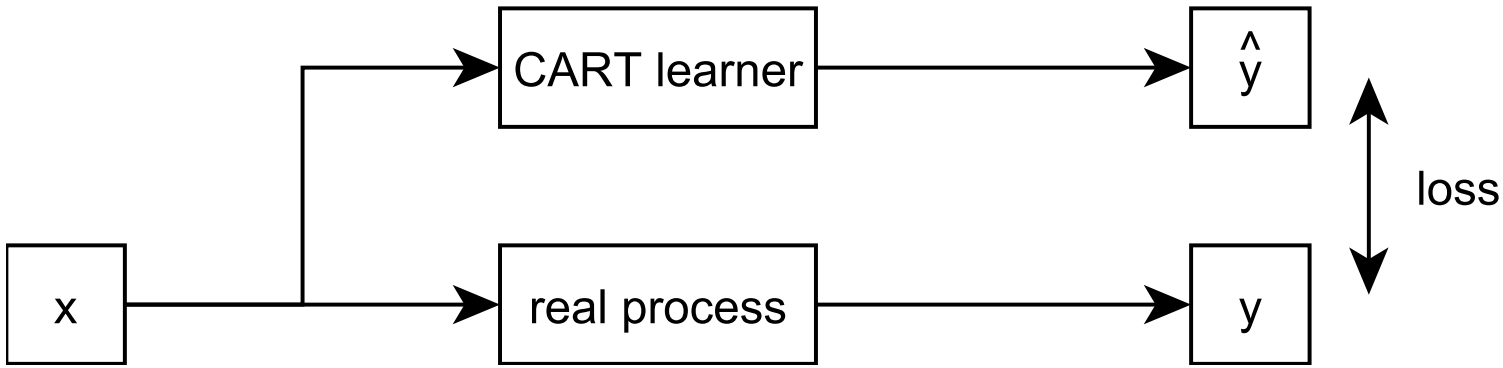
$\hookrightarrow$ What is $\mathcal{F}$? How to select f?

Supervised learning

- The set $\mathcal{F}$, called **the hypothesis space**:
  - depends on the learning method used
    ex: linear regression, $f(x) = ax + b$ with a, b the parameters of f
  - learn f means learn the parameters of the kind of function chosen
- The best f to select:
  - need of a tool that could measure the quality of the learned f
  - **objective function**, **loss function**, **risk function** (expectation of the loss)
  - risk function allows to **measure the error** made when we use the learned f
- **During the learning process** we use at each step a loss function: we want to **learn f under the constraint of a minimal loss**

Decision Tree: a supervised learner

- Decision tree is a supervised learning method
- It is also called CART (Classification And Regression Trees)



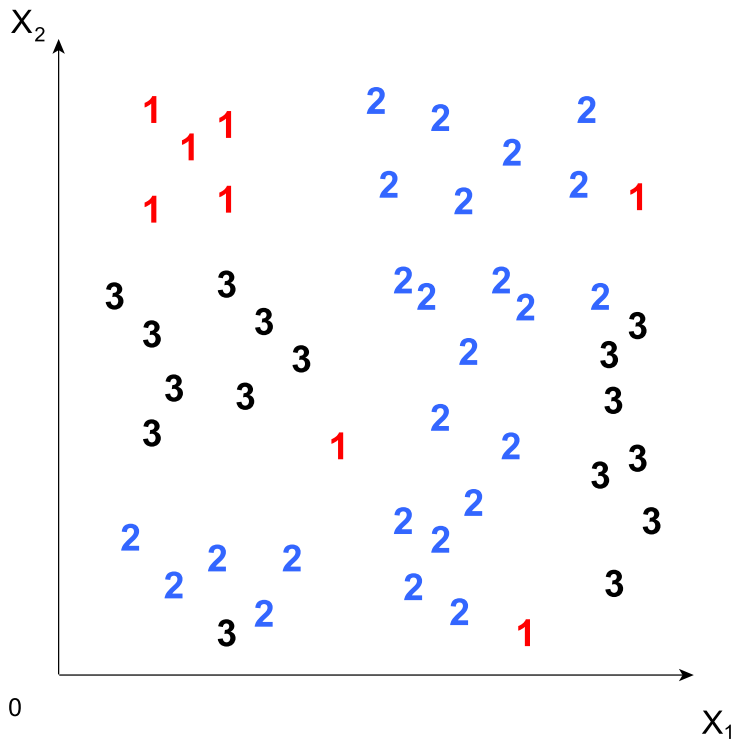
- To characterize Decision Tree method we have to answer,
  - What is $\mathcal{F}$?
  - How to learn the best f from $\mathcal{F}$?

Let's start by an illustration: a basic example

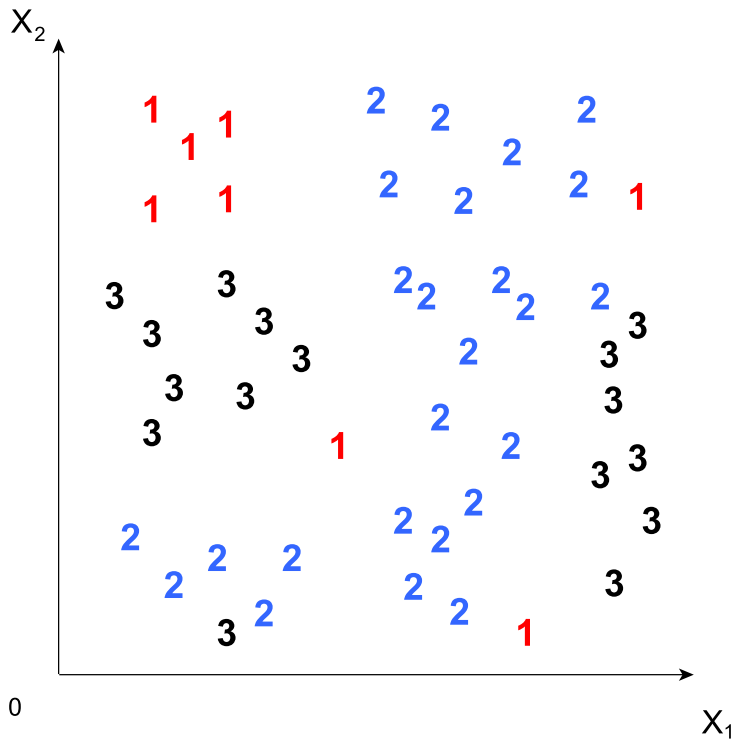
Plan

Example of a basic DT: case of a basic classification

- Learning set
  $\mathcal{D} = \left\{ \left(\left(x_{1,1}, x_{1,2} \right), y_1 \right), \ldots, \left(\left(x_{n,1}, x_{n,2} \right), y_n \right) \right\} \subset \mathbb{R}^2 \times \mathcal{Y}$
  where $x_i = \left(x_{i,1}, x_{i,2} \right) \in \mathbb{R}^2$ and $y \in \mathcal{Y} = \{1, 2, 3\}$



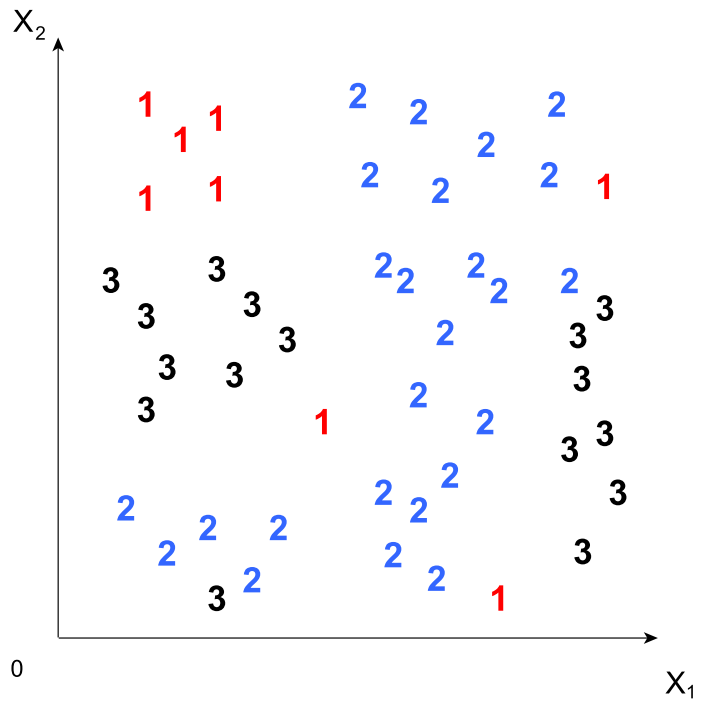
Example of a basic DT: case of a basic classification



- Problematic: segment $\mathbb{R}^2$ in pertinent classes using $\mathcal{D}$
- Goal: predict for each (new) x the well associated class
- Assumptions: the learning set $\mathcal{D}$ is representative and x_i are iid

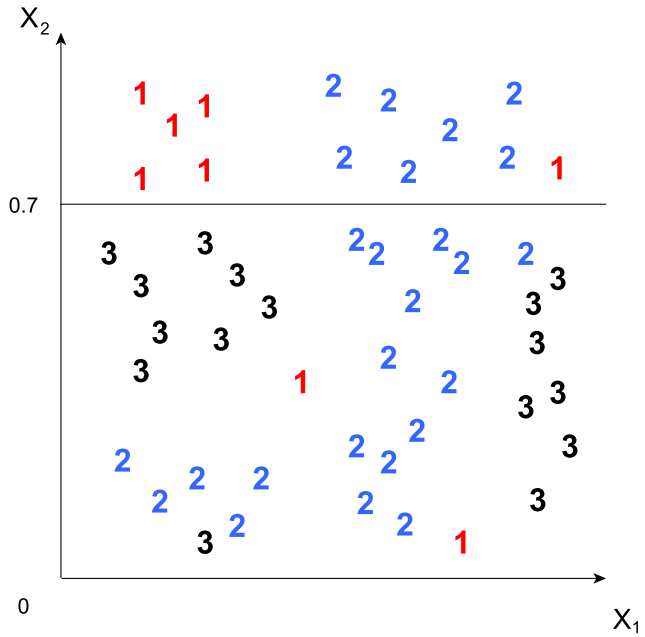
A basic DT building and the hypothesis space

- We can't see any kind of "line" $\rightarrow$ ~~linear model~~
- We need another and more appropriate hypothesis space



A basic DT building (the root)

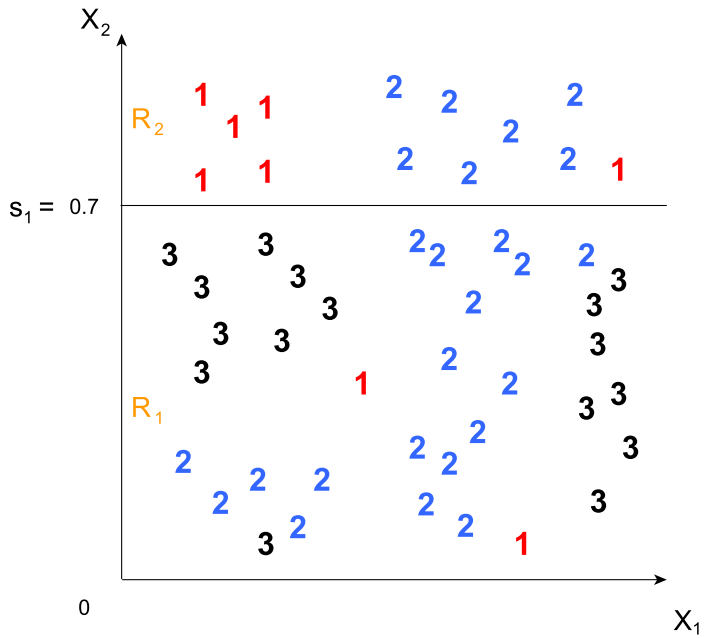
CART is an appropriate model that proceeds by using a recursive binary partition to isolate each class region

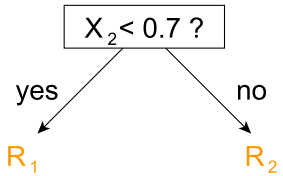


$X_2 < 0.7$?

- The horizontal line represents the decision boundary of the root node (depth 0): $X_2 = 0.7$

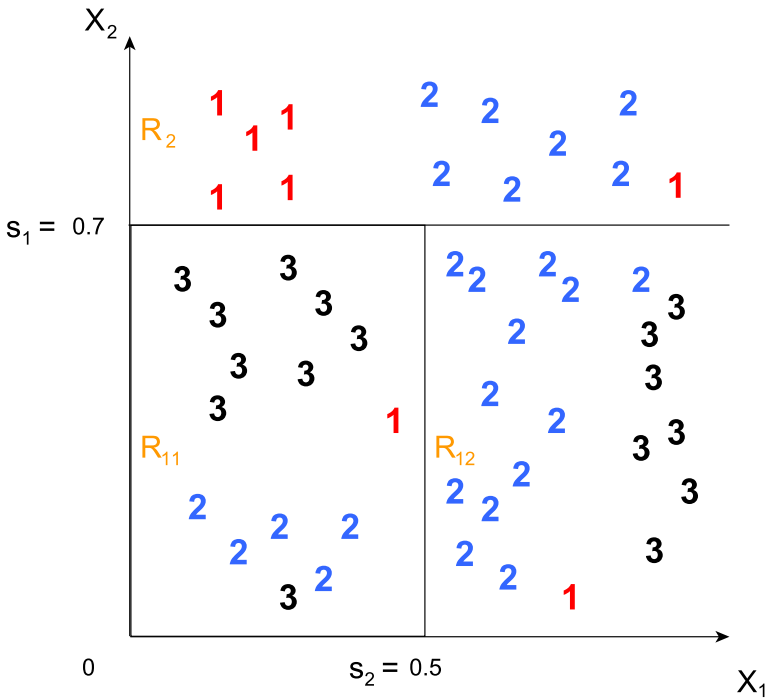
A basic DT building (depth = 1)

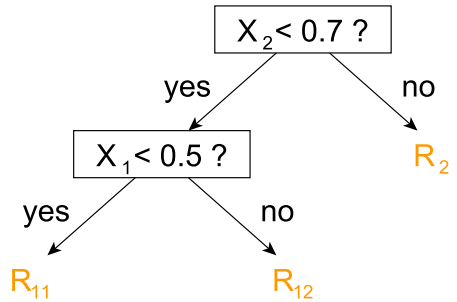




- However, the R_1 and R_2 areas are impure, so that we will grow a depth-2

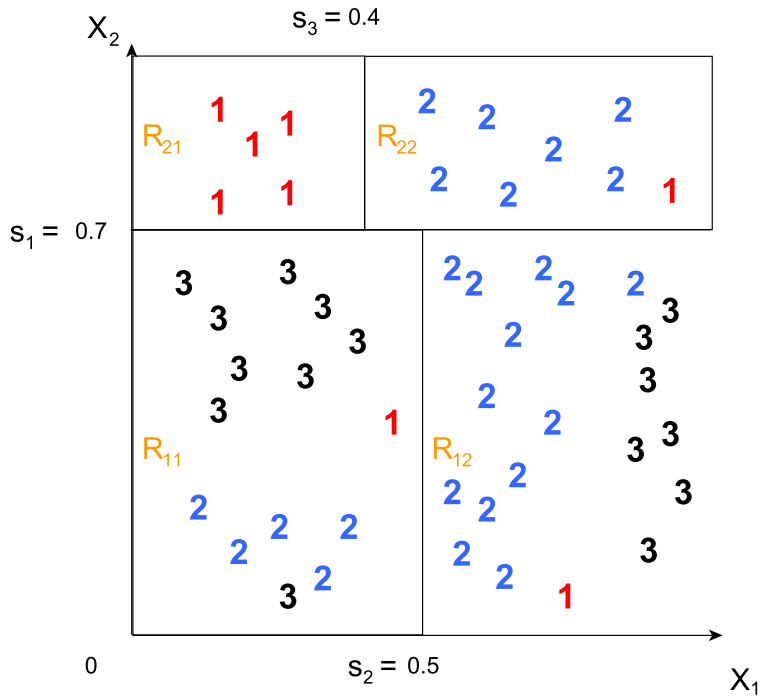
A basic DT building (depth = 2)

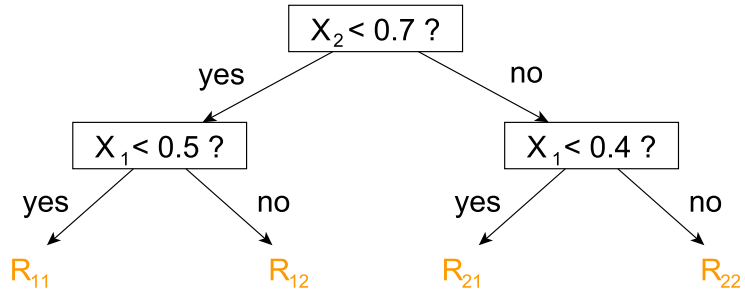




- Start spliting R_1: the depth-1 left node splits it at $X_1 = 0.5$ represented by the vertical segment

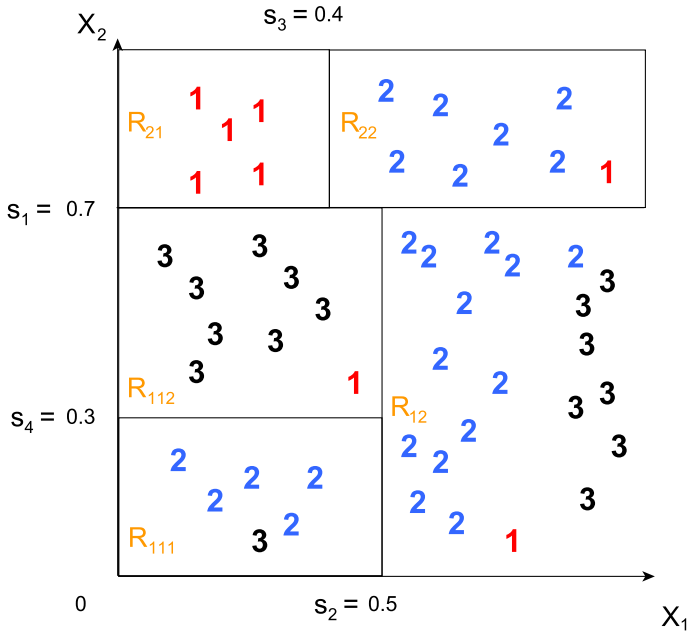
A basic DT building (depth = 2)

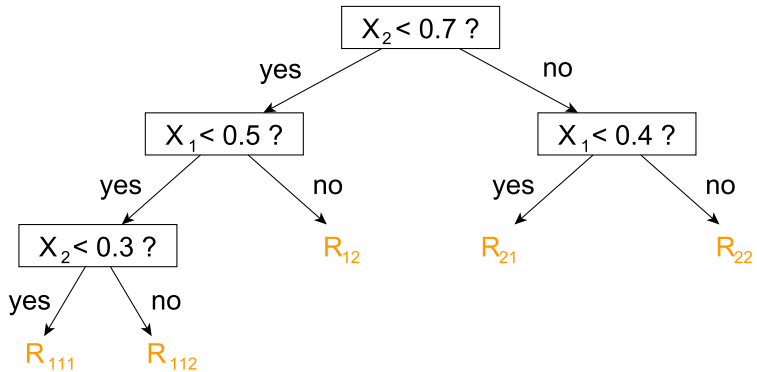




- Similarly, R_2 is split: the depth-1 right node splits it at $X_1 = 0.4$ represented by the upper vertical segment
- The two upper regions are pure enough; it won't be split any further
- However, the down regions are still impure

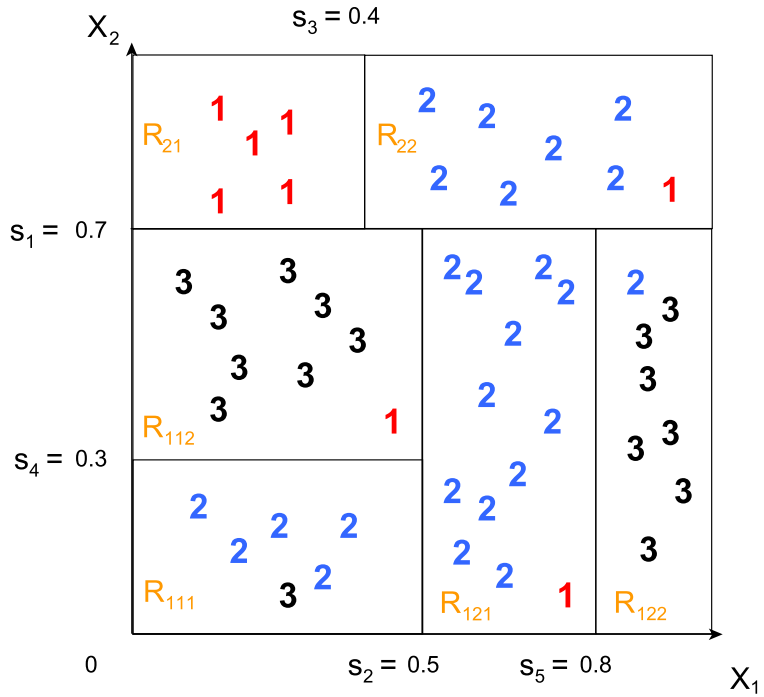
A basic DT building (depth = 3)

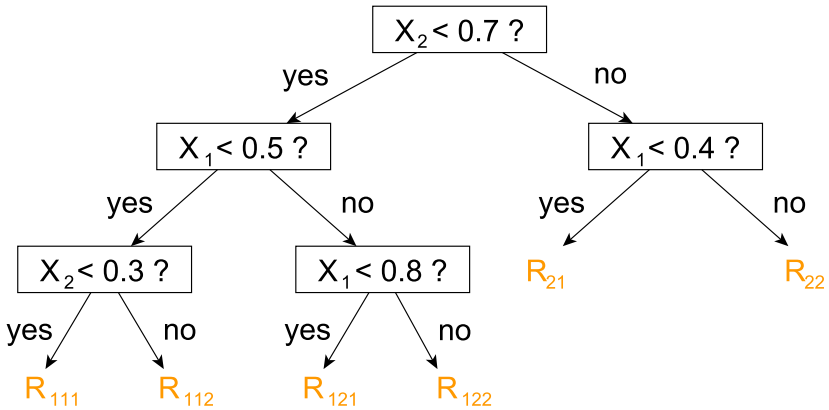




- The depth-2 left node splits it at $X_2 = 0.3$
- i.e. the region R_{11} is split and a new horizontal segment appears giving two regions R_{111}, R_{112} pure enough
- However, the down-right region R_{12} needs another split

A basic DT building (depth = 3)





- The depth-2 right node splits it at $X_1 = 0.8$
- i.e. the region R_{12} is split and a new vertical segment appears giving two regions R_{121}, R_{122} pure enough

A basic DT building (depth = 3)

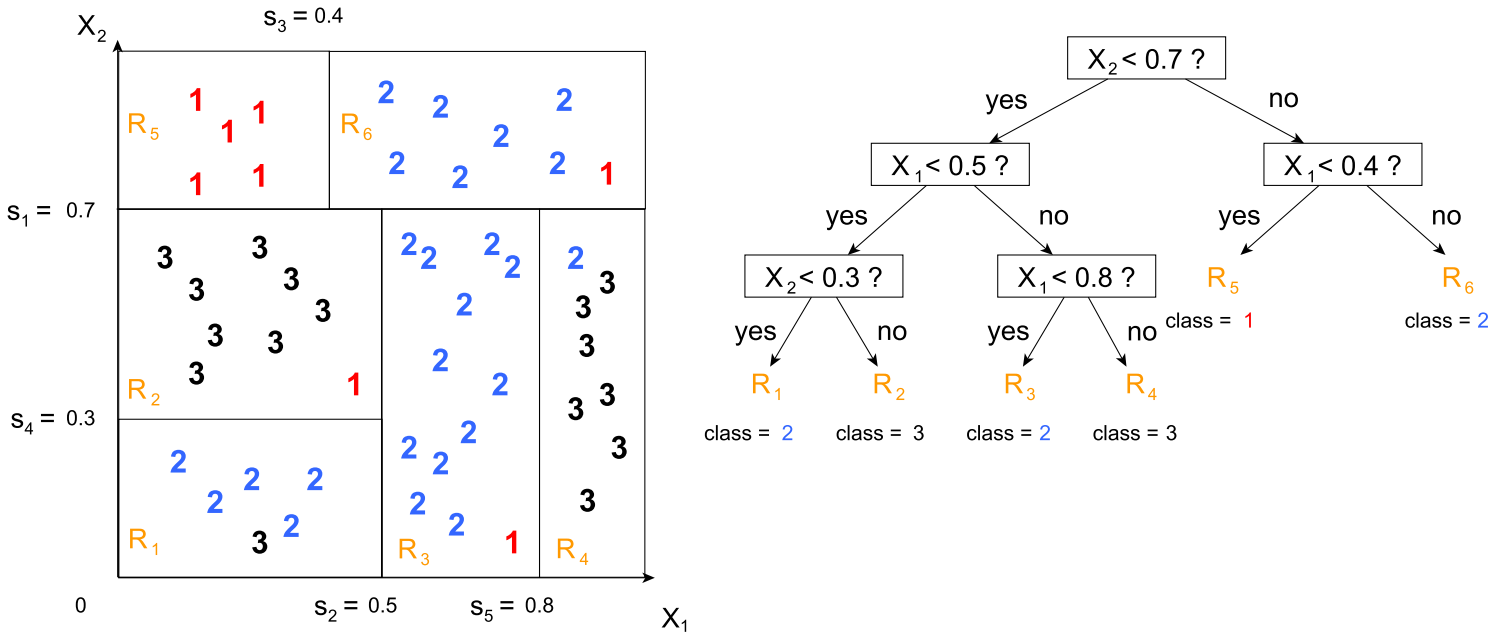


Figure: A classification tree predicting labels on a two-dimensional input space (left: the spatial segmentation, right: the visualized tree).

- The DT stops right there
- In practical case, you can parameterize the "pure enough" concept by setting "`max_depth`=3"
- We will introduce multiple stopping criterion

The basic DT obtained

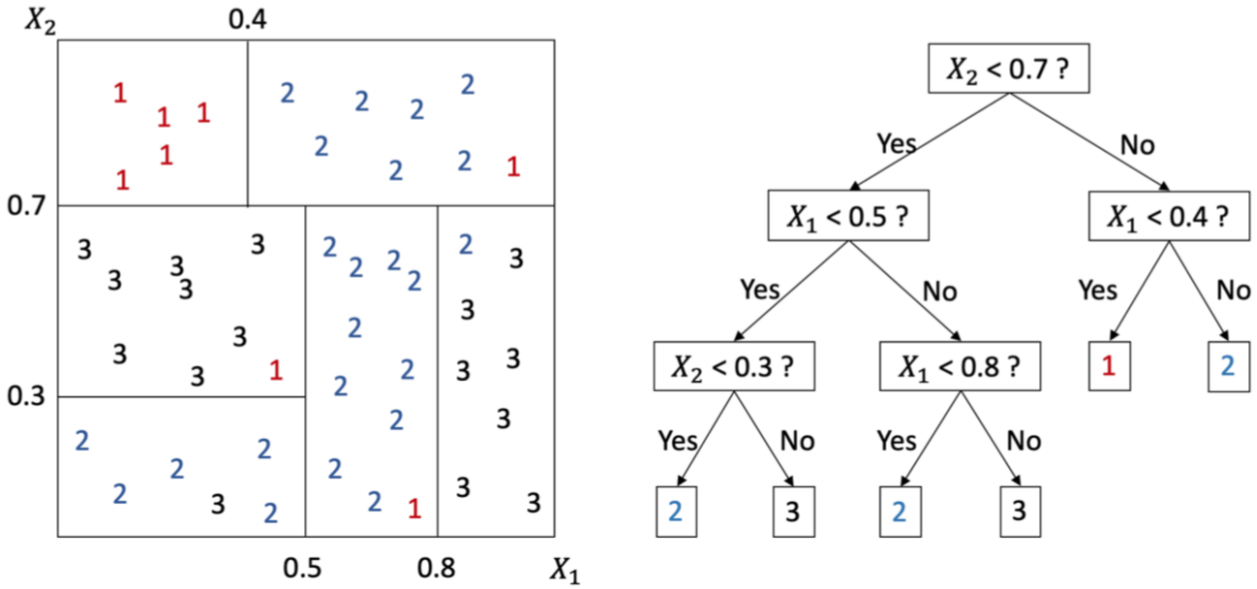
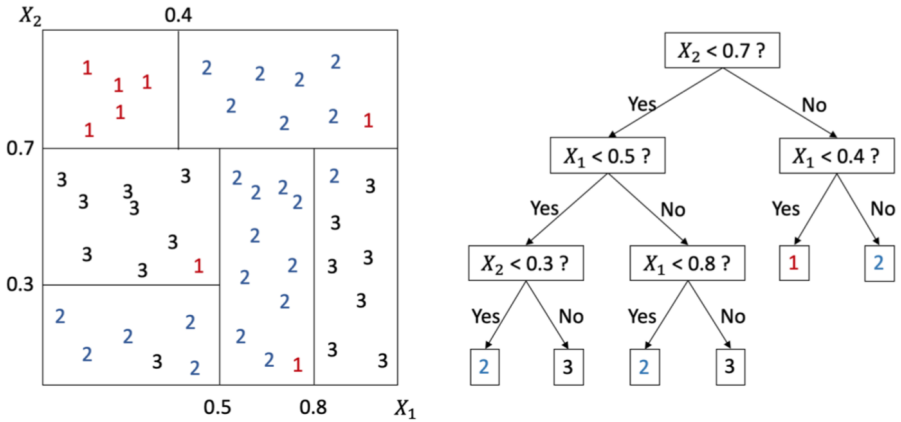


Figure: A classification tree predicting labels on a two-dimensional input space (left: the spatial segmentation, right: the visualized tree). Source: [Zhou, 2019].

- CART provides a partition of $\mathbb{R}^2$ in classes by horizontal/vertical line segments

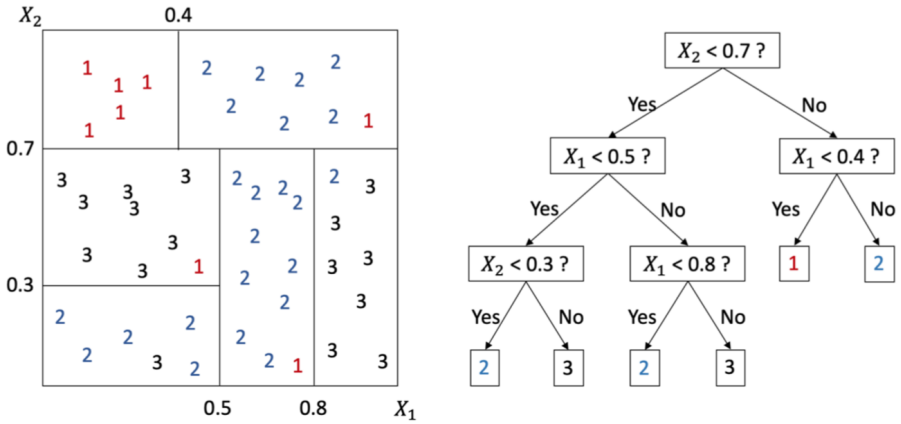
How this DT makes predictions?

Suppose you have a new x_{new} instance and you want to classify it



1. You start at the root node (depth 0, at the top): this node asks whether x_{new} has a X_2 value smaller than 0.7
2. If it is not, then you move down to the root's right child node (depth 1, right)
3. This is not a leaf node $\Rightarrow$ It asks another question: Is the X_1 value of x_{new} smaller than 0.4?
4. If it is, then x_{new} is most likely in the class 1. If not, it is likely in the class 2.

How estimate the class probabilities of an instance?



1. First, the instance traverses the tree to find the leaf node for it
2. It returns the ratio of training instances of each class c in this node

E.g., $x_i = (0.45, 0.05)$: the corresponding leaf node is the depth-3 left node (R_1)
So, DT should output the probabilities: 0 for the class 1, 5/6=0.83 for the majority class 2 and 1/6=0.17 for the class 3

Of course, DT predicts the class 2 for x_i

Model interpretation: white box versus black box

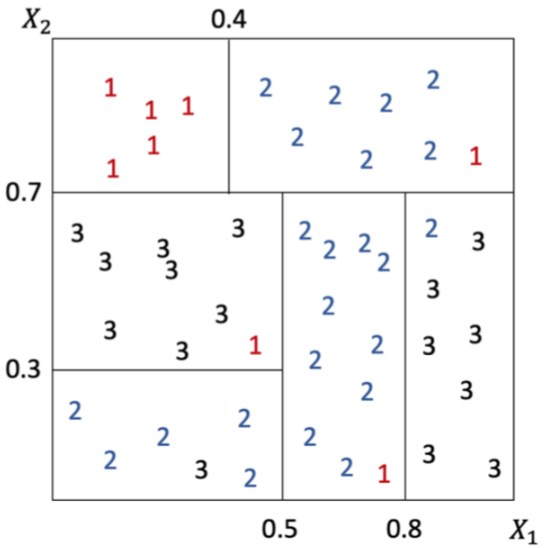
- As you can see DTs are intuitive and their decisions are easy to interpret!
- Such models are often called white box models
- In contrast, as we will see in next a lecture, Random Forests are generally considered black box models
- Black box models make great predictions, but it is usually hard to explain in simple terms why the predictions were made

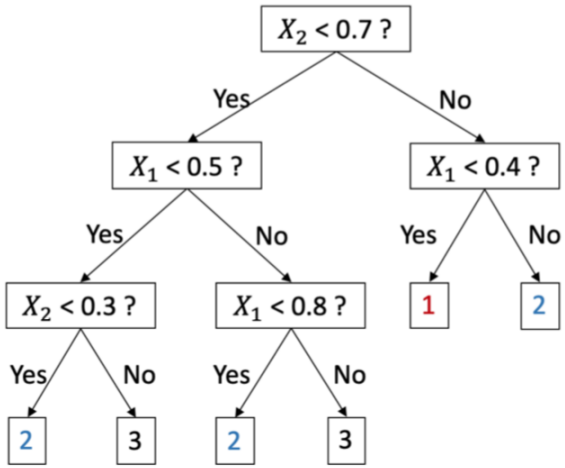
  E.g., if a neural network says that a particular person appears on a picture, it is hard to know what actually contributed to this prediction: did the model recognize that person's eyes? Her nose?
- Conversely, DTs provide nice and simple prediction rules that can even be applied manually if need be

Vocabulary used and to use

- Partitioning has a simple description like $X_2 = s_1$
- s_1, s_2, s_3, s_4, s_5 are the five **splits**
- Each **node** of the tree is characterized by a split and represent a **region**
- We have 6 final regions $R_1, R_2, R_3, R_4, R_5, R_6$
- The first node is called the **root**
- The two following nodes
  - are the **left and right childs**
  - are located at the **depth**=1 of the tree
- The final regions are called **leaves** (or terminal nodes) and give the final partition of the **feature space**
  $\mathcal{X} = R_1 \cup R_2 \cup R_3 \cup R_4 \cup R_5 \cup R_6$

The prediction rule





- The structure of the learned DT gives the classification rule
- It's formula is the function $\hat{f}$ learned to be as close as possible to f

Exercise 1

Write the $\hat{f}(x)$ formula associated to the classification tree example?

Vocabulary and conventions

- A decision tree is characterized by the regions partitioning $\mathcal{X}$ and the classes (or values) predicted for each region

Exercise 2

Rewrite $\hat{f}(x)$ formula with the regions $R_1, R_2, R_3, R_4, R_5, R_6$?

Exercise 3

Rewrite $\hat{f}(x)$ formula with a sum symbol from $k = 1$ to $k = K = 6$?

Remark: k also indexes the nodes

Decision tree model

Definition (Decision tree)

A decision tree is a binary tree that recursively segment the input space $\mathcal{X}$, also called the feature space, along the coordinate directions to create a set of K hyper-rectangles R_k, $k \in \{1, \ldots, K\}$ as basic prediction units for fitting constant values γ_k within each of them. The decision tree model is formulated as follow:

$$f(x) := \sum_{k=1}^{K} \gamma_k \mathbb{1}_{\{\boldsymbol{x} \in R_k\}} \tag{1}$$

where $x \in \mathcal{X}$ and γ_k the corresponding predicted value or class for the dependent variable (called also output variable and denoted Y).

We call γ_k and R_k the “parameters" of the DT model.

Parameters of a decision tree model

Elements of intuition:

- The set of K hyper-rectangles R_k is determined by a set of $K-1$ chosen splits and their order during the recursive binary segmentation
- Each split is determined by a greedy strategy to best discriminate the observations in its two branches respectively
- The fitted value γ_k assigned to each terminal node R_k is usually decided by the majority vote (classification task) or the average (regression task)
- Several decision tree models are possible: as much as input space partitions and set of γ_k (instability)

Parameters of a decision tree model

- We speak about DT as no-parametric model
- It's not because it does not have any but because the number of parameters is not determined prior to training
- So the model structure is free to stick closely to the data
- Conversely, a linear model is a parametric one with parameters allowing to don't stick closely to the data

That's why DT come from the no-parametric models family but have parameters

How estimate the parameters of a DT model

- We wish the best decision tree predictor $\hat{f}(x) = \sum_{k=1}^{K} \hat{\gamma}_k \mathbb{1}_{\{\boldsymbol{x} \in \hat{R}_k\}}$
- In practice, this is realized by minimizing a given **risk function** or **impurity measure** (this is called the main optimization problem)
- Allowing to evaluate the error made by the learning predictor

Definition (Risk function)

$$\mathcal{R}(f) := P(y \neq f(x))$$

Examples of risk function (Classification case)

- $\mathcal{R}_n(f) := \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{y_i \neq f(x_i)\}}$ is the empirical misclassification loss
- The misclassification loss is illustrated bellow with another losses

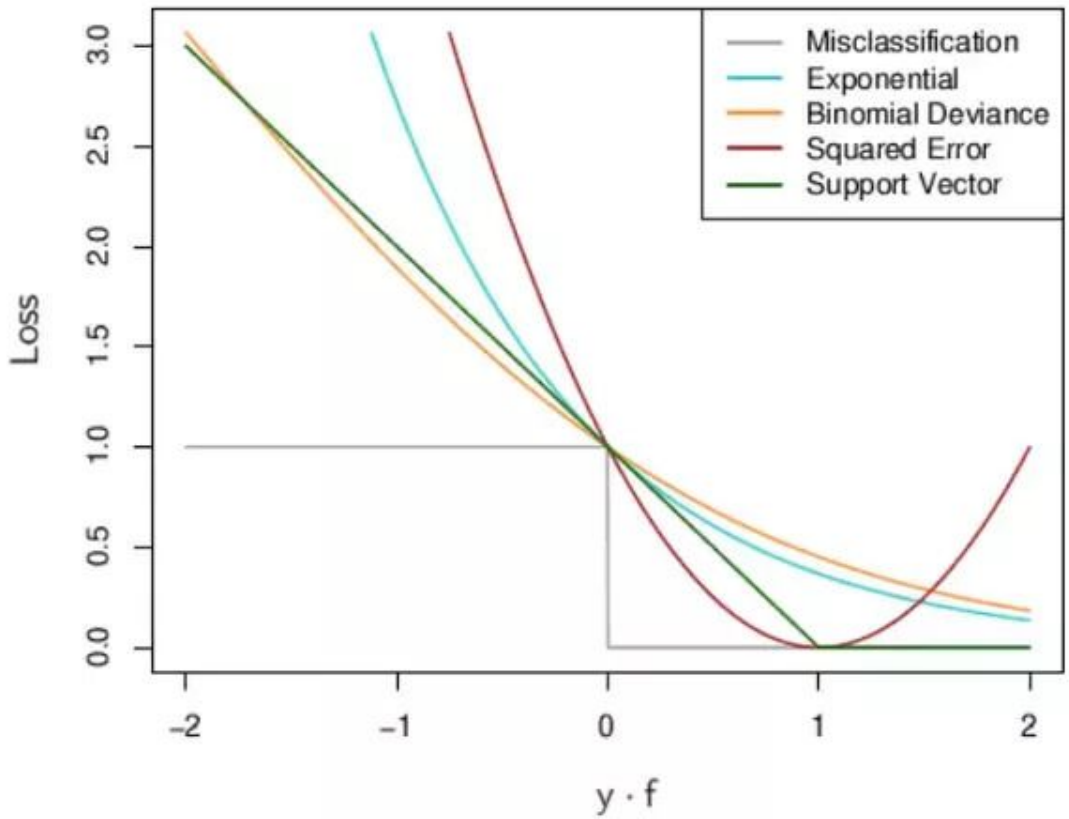


Figure: Illustration of some losses for binary classification

Examples of risk function (Regression case)

Definition (L2 loss - Squared Loss)

$\mathcal{R}_n(f) := \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$ is the empirical and squared loss also called L2-loss.

Each empirical risk has a no-empirical formula:
$\mathcal{R}(f) := \int_{\mathcal{X}\times\mathcal{Y}}(y - f(x))^2\, dP(x, y)$ is the squared loss

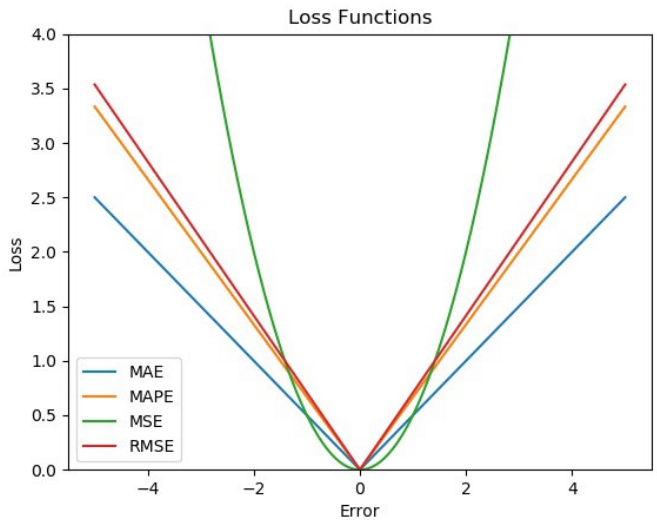


Figure: Illustration of some popular losses for regression

Building a regression DT

- The minimization of the risk function allows the construction of a decision tree by determining the best values for the sets of R_k and γ_k
- Given a learning set $\mathcal{D} = \left\{(x_i, y_i)_{1 \leqslant i \leqslant n}\right\} \subset \mathcal{X} \times \mathcal{Y}$ and using the empirical quadratic risk function, one should solve:

Optimization problem (empirical case)

$$\min_{\gamma_1,\cdots,\gamma_K,R_1,\cdots,R_K} \mathcal{R}_n(f) = \min_{\gamma_1,\cdots,\gamma_K,R_1,\cdots,R_K} \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$$

- Another version of optimization problem:

$$\min_{\gamma_1,\cdots,\gamma_K,R_1,\cdots,R_K} \mathbb{E}\left[(y_i - f(x_i))^2\right]$$

Building a regression DT: predictive rule

Let's solve the optimization problem (γ_k case)

$$\min_{\gamma_1,\cdots,\gamma_K} \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \sum_{k=1}^{K}\gamma_k \mathbb{1}_{\{x_i \in R_k\}}\right)^2$$

$\forall k \in \{1,\ldots,K\}$,

$$\hat{\gamma}_k = \underset{\gamma_k}{\text{argmin}} \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \gamma_k \mathbb{1}_{\{x_i \in R_k\}}\right)^2 \text{ (disjoint regions)}$$

$\forall k \in \{1,\ldots,K\}$, given $x_i \in R_k$,

$$\hat{\gamma}_k = \underset{\gamma_k}{\text{argmin}} \frac{1}{n}\sum_{i:x_i \in R_k}^{n}\left(y_i - \gamma_k\right)^2$$

Then, $\forall k \in \{1,\ldots,K\}$, given $x_i \in R_k$,

$$\frac{\partial}{\partial \gamma_k}\mathcal{R}_n(f) = 0 \Leftrightarrow \sum_{i:x_i \in R_k}^{n} -2\left(y_i - \gamma_k\right) = 0 \text{ (formula derivates)}$$

$$\Leftrightarrow \hat{\gamma}_k = \frac{1}{|R_k|}\sum_{i:x_i \in R_k}^{n} y_i \quad \text{given } x_i \in R_k$$

Building a regression DT: predictive rule

Thus, we obtain

the predictive rule

For each $x_i \in R_k \Longrightarrow \hat{f}(x_i) = \frac{1}{|R_k|} \sum_{i=1}^{n} y_i \mathbb{1}_{\{x_i \in R_k\}}$

- This is the empirical expectation of outputs corresponding to inputs belonging to region R_k

Notations,

$$\hat{\gamma}_k = \frac{1}{|R_k|} \sum_{i=1}^{n} y_i \mathbb{1}_{\{x_i \in R_k\}}$$

$$\Leftrightarrow \hat{\gamma}_k = \frac{\sum_{i=1}^{n} y_i \mathbb{1}_{\{x_i \in R_k\}}}{\sum_{i=1}^{n} \mathbb{1}_{\{x_i \in R_k\}}}$$

$$\Leftrightarrow \hat{\gamma}_k = average\,(y_i | x_i \in R_k)$$

Building a regression DT: split rule

- Finding the best binary partition in the term of risk $\mathcal{R}_n$ is more complicated $\Rightarrow$ proceed with a greedy algorithm
- Let j be a splitting variable (index of feature x^j from the input), s a split point and define the pair of half-planes

$$R_1(j,s) = \left\{x_i \in \mathcal{D} : x_{i,j} \leqslant s\right\} \text{ and } R_2(j,s) = \left\{x_i \in \mathcal{D} : x_{i,j} > s\right\}$$

- Then, we search for the couple (j,s) that produces the purest subsets, i.e., solving,

Definition (CART cost function for regression)

$$\min_{j,s}\left[\min_{\gamma_1}\sum_{x_i\in R_1(j,s)}(y_i-\gamma_1)^2+\min_{\gamma_2}\sum_{x_i\in R_2(j,s)}(y_i-\gamma_2)^2\right] \tag{2}$$

where, for any choice of (j,s), the inner minimization is solved by

$$\hat{\gamma}_1 = \textit{average}\left(y_i | x_i \in R_1(j,s)\right) \text{ and } \hat{\gamma}_2 = \textit{average}\left(y_i | x_i \in R_2(j,s)\right)$$

Building a regression DT: split rule

- To compute $\hat{\gamma}_1$ and $\hat{\gamma}_2$ we need to determine $R_1(j, s)$ and $R_2(j, s)$, ie: the couple (j, s)

The splitting process of one region in two child regions

- We scan each dimension of all the inputs $j \in \{1, \ldots, d\}$ and each $n - 1$ split points for each fixed j
- For each split (j, s) we compute the risk value thanks to $\hat{\gamma}_1$ and $\hat{\gamma}_2$ formula
- We stock smartly the risk values computed for each couple (j, s)
- Choose the couple (j, s) that associated to the minimal risk value
- Partition the data into the two resulting regions

- This splitting process is repeated for each child regions, and so on
- That's why we call it a "greedy" process

Building a regression DT: stopping criterion and pruning

How much should we let the tree grow?

- Too big a tree may **overfit** the data
- Too small a tree risk of **not capturing their structure**
- The optimal size is a **hyper-parameter to calibrate** on the data

Solutions:

- Grow as long as the variance within the leaves decreases more than a fixed threshold
  Too short-term vision: a bad cut can sometimes lead to very good cuts
- **Pruning:** we make the tree grow to the maximum and then we remove the uninteresting nodes.

Building a regression DT: stopping criterion

- The repetition is made until a stopping criterion is met
- To avoid overfitting the training data, you need to restrict the DT's freedom during training
- Examples of stopping criterion or "regularization by setting hyperparameters",
  - maximum depth
  - maximum number of leaves
  - minimum number of sample per leaf
- They can help to avoid overfitting by avoiding, to grow the maximal tree that overfits the training data

Suggestion: During the lab or at home, try to observe it with moon dataset:

```
from sklearn.datasets import make_moons
```

Building a DT: pruning

Another way to avoid overfitting
We re-examine the tree and remove the nodes caused by the noise present in the learning set

Penalized criterion

- The optimal tree is a pruned subtree **minimizing** the prediction error penalized by the complexity of the model (length of the tree) $|T|$,

$$\mathcal{R}_\alpha(f_T) = \mathcal{R}_n(f_T) + \alpha \frac{|T|}{n}$$

  $\mathcal{R}_n(f_T)$ is the error term linked to the decision subtree f_T (ex: Mean Squared error or the rate of misclassifications)
- The complexity parameter $\alpha \in [0, 1]$ penalizes large trees

Evaluate a regression DT model

- The decision tree is learned on the **learning set**
- Hyper-parameters could be calibrate on a **validation set**
- To evaluate the accuracy, we could compute the error made on a **test set** via an error measure (MSE is the most popular for regression)

  MSE (Mean Squared Error) is a metric which looks like the L2 squared loss (risk function we saw before), corresponding to the expected value of the squared error loss,

$$\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{f}(x_i)\right)^2$$

- Usually, a 5-fold cross validation process is realized on the data set

Summary: the greedy building of a regression DT

CART algorithm [Breiman et al., 1984]

1. Start at the root node corresponding to the full input space $\mathcal{X}$
2. Given a node, enumerate all possible candidate splits by going over all features and collecting all possible split values
3. Choose a split solving the optimization problem (2) to separate the node, thus the corresponding feature sub-space, into two child branches
4. Work recursively in the child node to further split until a stopping criterion is met
5. Calculate the fitted value in each of the terminal nodes

This algorithm is generic to classification DT by adapting the optimization problem

Plan

Building a classification DT: Formalization

- Output variable: $y \in \mathcal{Y} = \{1, \ldots, c, \ldots, C\}$, C classes
- Learning set $\mathcal{D} = \left\{(x_i, y_i)_{1 \leqslant i \leqslant n}\right\} \subset \mathcal{X} \times \mathcal{Y}$

Proportion of class c observations in a node k

For a node k representing a region R_k with $n_k = \sum_{i=1}^{n} \mathbb{1}_{\{x_i \in R_k\}}$ data points, we define:

$$\hat{p}_{k,c} := \frac{1}{n_k} \sum_{x_i \in R_k} \mathbb{1}_{\{y_i = c\}}$$

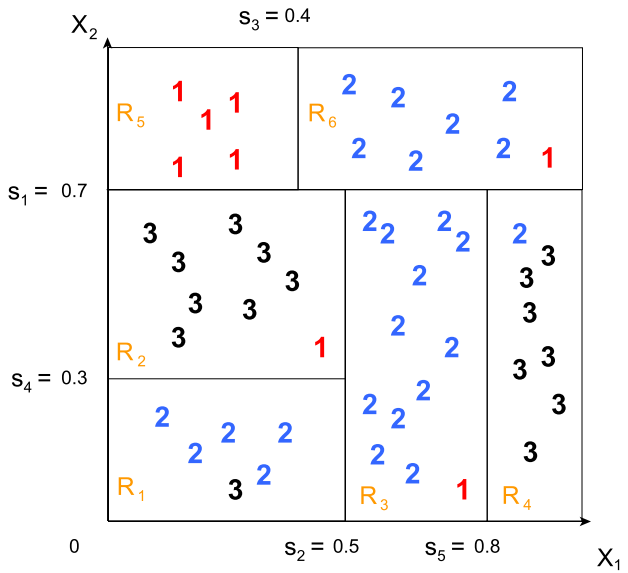
the proportion of class c observations in node k

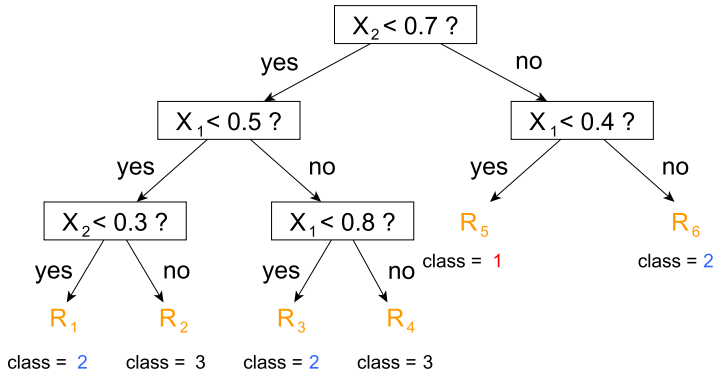
Classification rule (majority vote)

We classify the observations in node k to class $c(k)$ such as

$$c(k) := \underset{1 \leqslant c \leqslant C}{\operatorname{argmax}}\, \hat{p}_{k,c} \qquad \text{(the majority class)}$$

Illustration of the classification rule





- The proportion of class $c = 1$ observations in node $k = 1$ is $\hat{p}_{1,1} = \frac{1}{6} \sum_{x_i \in R_1} \mathbb{1}_{\{y_i = 1\}} = 0$
- For $c = 2$, we have $\hat{p}_{1,2} = \frac{1}{6} \sum_{x_i \in R_1} \mathbb{1}_{\{y_i = 2\}} = 5/6$
- For $c = 3$, we have $\hat{p}_{1,3} = \frac{1}{6} \sum_{x_i \in R_k} \mathbb{1}_{\{y_i = 3\}} = 1/6$

The classification rule is given by the majority class,

$$c(1) = \underset{1 \leqslant c \leqslant C}{\operatorname{argmax}}\, \hat{p}_{1,c} = 2$$

Building a classification DT

- Let's write $\mathcal{D}_k$ the data points in a node k,

$$\mathcal{D}_k = \{(x_i, y_i) \in \mathcal{D} : x_i \in R_k\}$$

- We consider risk functions addapted to classification
- To split nodes, we want to choose a **split yielding a maximal impurity reduction** to solve the optimization problem
- Several measures $\mathcal{Q}(\mathcal{D}_k)$ of node impurity can be considered
  - **Misclassification error**

$$\mathcal{Q}(\mathcal{D}_k) = \frac{1}{n_k} \sum_{x_i \in R_k} \mathbb{1}_{\{y_i \neq c(k)\}} = 1 - \hat{p}_{k,c(k)} \tag{3}$$

  - **Gini index**

$$\mathcal{Q}(\mathcal{D}_k) = \sum_{c \neq c'} \hat{p}_{k,c} \hat{p}_{k,c'} = \sum_{c=1}^{C} \hat{p}_{k,c}(1 - \hat{p}_{k,c}) \tag{4}$$

  - **Cross-entropy**

$$\mathcal{Q}(\mathcal{D}_k) = - \sum_{c=1; \hat{p}_{k,c} \neq 0}^{C} \hat{p}_{k,c} \ln(\hat{p}_{k,c}) \tag{5}$$

Building a classification decision tree

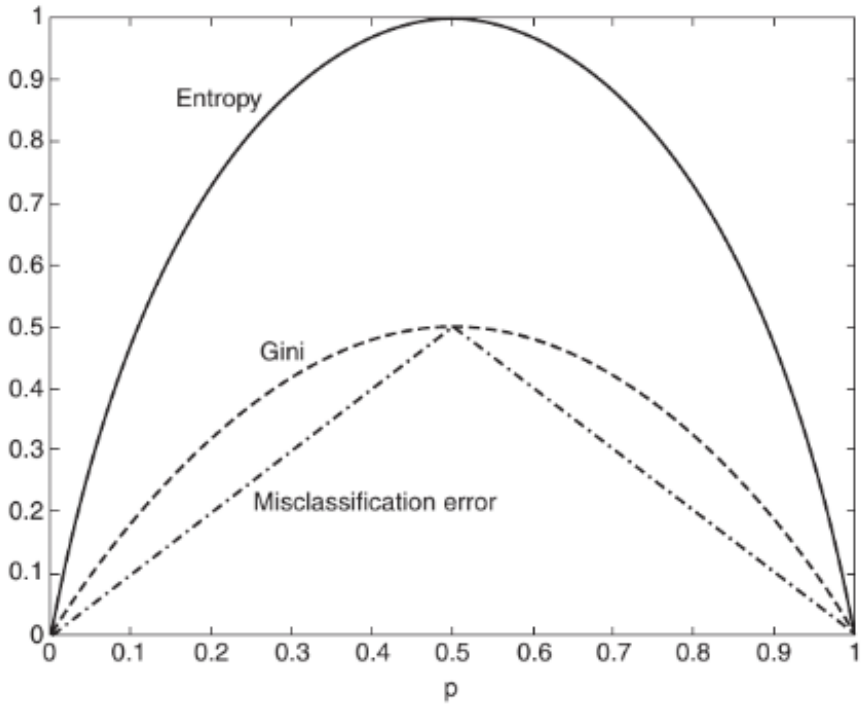


Figure: Illustration of node impurity measures (binary classification case), as a function of the proportion p in one class

- We don't want to be in the situation where two observations are affected to two different classes with the same probability 0.5 (as random)

Building a classification DT: Gini or Cross-entropy?

- Most of the time it does not make a big difference and lead to similar trees
- Gini impurity is slightly faster to compute $\Rightarrow$ it is a good default
- However, when they differ, Gini impurity tends to isolate the most frequent class in its own branch of the tree, while entropy tends to produce slightly more balanced trees

Building a classification tree: split rule

The tree is grown as per the regression tree presented before

- A region R_k is given
- Consider a couple (j, s) of splitting variable and split point
- Let's write $\mathcal{D}_{k,L}(j, s)$ the resulting data set of left node of size $n_{k,L}$ and $\mathcal{D}_{k,R}(j, s)$ for the right node, of size $n_{k,R}$
- The tree is growing by solving the following optimization problem,

Definition (CART cost function for classification)

$$\min_{j,s} \left\{ n_{k,L}\, \mathcal{Q}\left(\mathcal{D}_{k,L}(j,s)\right) + n_{k,R}\, \mathcal{Q}\left(\mathcal{D}_{k,R}(j,s)\right) \right\}$$

where $\mathcal{Q}()$ is one of the impurity measures (3),(4),(5)

Building a classification tree: stopping criterion, pruning, evaluation

All notions about

- stopping criterion
- pruning
- evaluation

presented previously are extendable to classification decision trees

The error measure used for the classification case is the misclassification error Eq. (3)

Several point of views of a decision tree

- Decision tree (DT) is a piece-wise constant estimate and a finite linear combination of hyper-rectangular indicators functions
- Among Lebesgue theory deeper is a DT, better is the accuracy
- DT is an adaptive nearest neighbor smooth where the distance measure between 2 points corresponds to the likelihood of them being in the same terminal node
- A DT is able to create a topology on the feature space describing the similarity between observations
- A DT is a combination of binary decision paths mimicking human decision, where a decision rule is a dichotomous evaluation (of if-then predicates)

Decision tree pros

- DT is a powerful machine learning tool without relying on structural assumptions regarding the underlying space
- DTs are interpretable predictors and easy to train
- DT can handle categorical values (binerazing them)
- DT can handle missing input values ([Hastie et al., 2009], chapter 9)

Decision tree cons

- The construction process is greedy (cf. DT's complexity in [Géron, 2017], chapter 6)
- CARTs are neither smooth, Liepshitz nor even continuous
- DTs are adaptive to training sample through their building algorithm
  $\rightarrow$ Analysis have to be conditioned by the learning data
- Thus, trees are **unstable**: DTs have a high variance
  $\rightarrow$ A small change on data can result on a different predictor
- A way to reduce the related variance: **ensemble methods**
  - Bagging
  - Random forests
  - Boosting

Random Forests can limit this instability by averaging predictions over many DTs, as we will see in the next lecture!

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