Decision Trees and Random Forests
Data science Certificate

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1. Decision Trees

2. Random Forests

- goal in ML
- how it is defined
- parameters
- implement it in Python.
- + / -

Outline

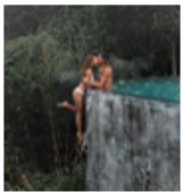
Random Forests

Supervised ML framework

- Task: do these pictures contain individuals that look nice (yes or no), suspicious (yes or no)?
- Train algorithms using data (a lot of these):







Nice: yes **Susp: no**

Nice: no **Susp: yes**

Nice: yes **Susp: yes**

Nice: yes **Susp: yes**

Nice: yes **Susp: yes**

each image $\in$ 1 category.

- Pictures: $X_i \in \mathbb{R}^d$, Labels $Y_i \in \{0, 1, 2, 3\}$ $\{0,1\}$
- Features: categorical and numerical features (is there a smile? what is the age of the person ?)
- Size of the dataset: n for training $+t$ for test.

Goals of Decision Trees

	age	weight	height	salary
Features :	25	65	1,8	1M
Learned :	2	-1	20	0,005

Price of house : not easily interpretable

Yesterday b_i weights

Today w_i weights

to learn

1. Prediction: what is the class of this picture (Classification) ? What is the age of the person (Regression) ?

2. Provide some understanding: what on this picture allows me to classify it? Ex: presence of a face, human, smiling, etc ...

image: has features $x_1^i \dots x_d^i$

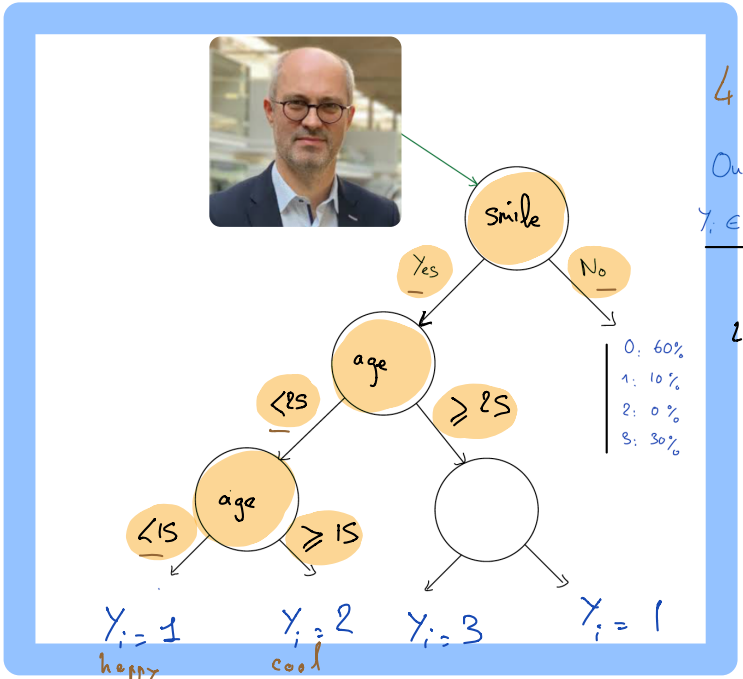
d nbr of features

linear regression: predict output y_i by $\sum_{i=1}^{d} w_i x_1^i$

Decision Tree

Training data : images and their features + category

- **Nodes** = tests
- **Branches** = possible outcomes
- **Leaves** = final decision.



4 categories.

Output label

$Y_i \in \{0,1,2,3\}$

Leaf

$Y_i = [0]$

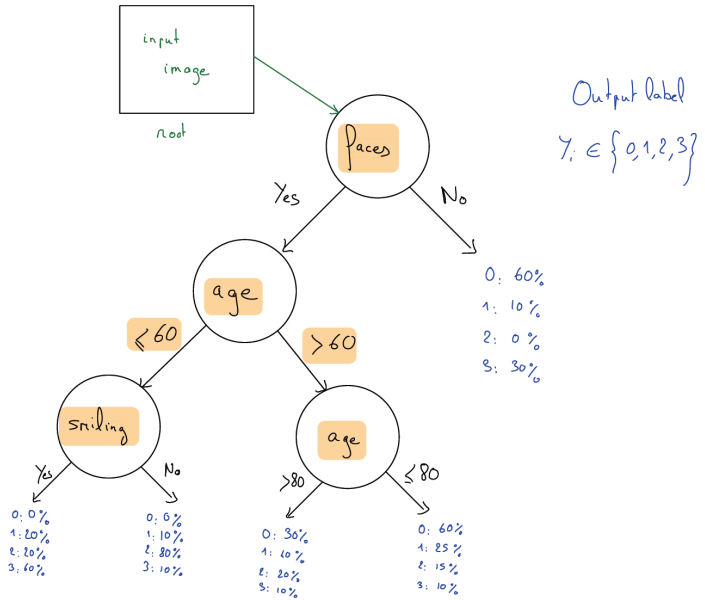
Learn : For each node:
- which feature to use
- decision criterion.

Output: * classification : category
* regression : continuous

↑ what you want to predict.

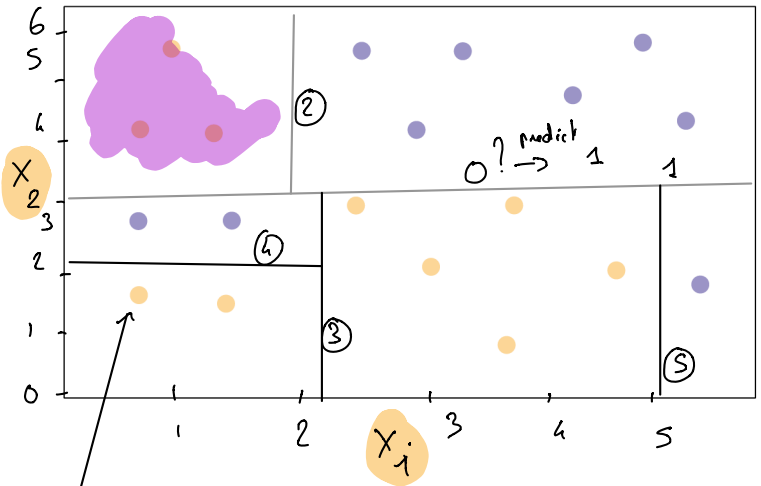
Decision Tree

- Nodes = tests
- Branches = possible outcomes
- Leaves = final decision.



Building trees : CART

↕ algo to learn tree



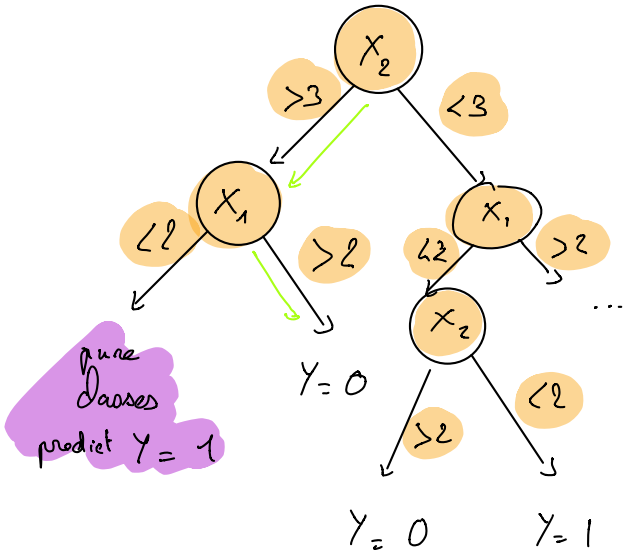
$Y_i = 0$ happy

$Y_i = 1$ no

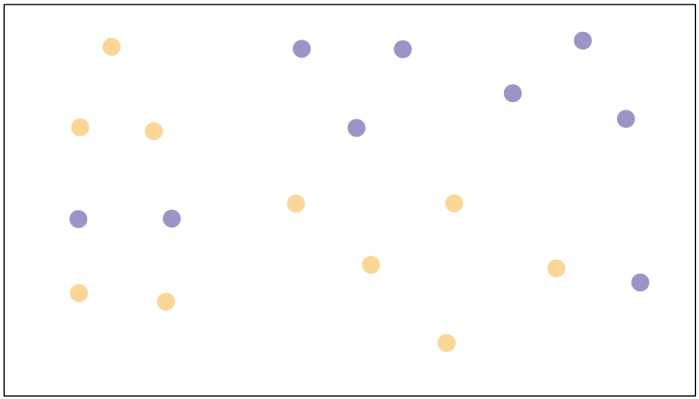
yes

obs n° 1 : (X_1^1, X_1^2), label "no" = 0

2 features input pt



Building trees : CART



$\bar{Y} = 0.5$: 0, 1

$\bar{Y} = 15.5$: 10, 21

average $\frac{32}{4} = 8$

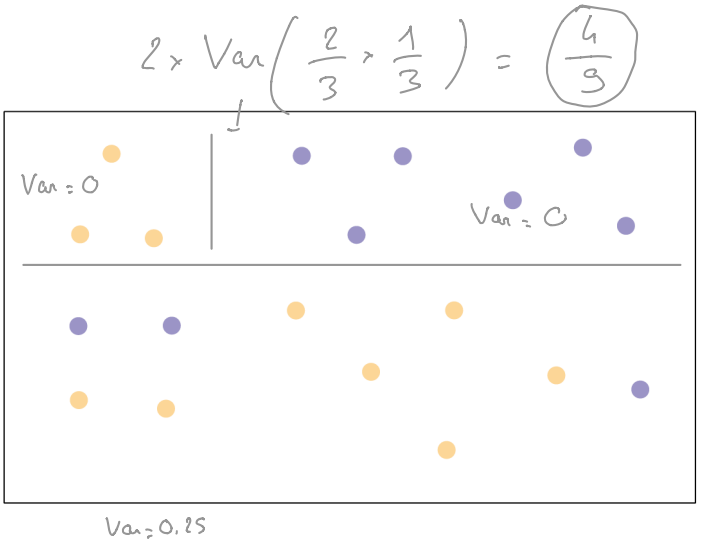
no split : $MSE = (0.8)^2 + (1-8)^2 + (10-8)^2 + (21-8)^2$

after split MSE : $(0-0.5)^2 + (1-0.5)^2 + (10-15.5)^2 + (21-15.5)^2$

How to chose the best cut ?

- e.g., Given a possible cut, measure the reduction of « impurity »:
  - in regression: mean-squared-error $\sum_{i \in C}(Y_i - \bar{Y}_C)^2$
  - in classification: Gini's impurity.
- Find dimension and threshold with optimal impurity reduction.
- Iterate until stopping criterion is met.

Gini's impurity



$2 \times Var\left(\frac{2}{3} \times \frac{1}{3}\right) = \frac{4}{9}$

9 blue pts

10 orange pts

Gini's impurity $\simeq 0.5$

For a pt in cat i, probability of misclassif $= (1 - p_i)$

Gini impurity measures **how often a randomly chosen element from the set** would be **incorrectly labeled if it was randomly labeled according to the distribution of labels in the subset**.

proba cat i — proba misclassif.

$$I_G(p) = \sum_{i=1}^{J} p_i(1 - p_i) = 1 - \sum_{i=1}^{J} {p_i}^2$$

For two classes, related to the variance if classified as Bernoulli r.v..

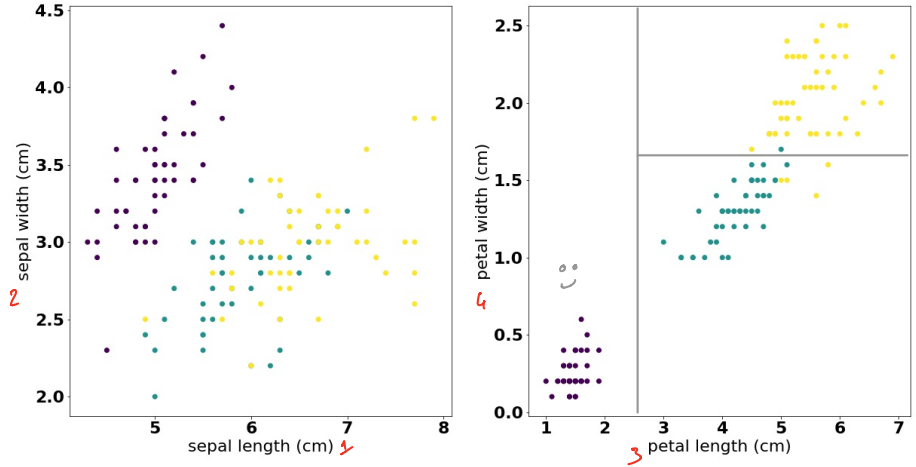
$Var\left(\mathcal{B}(p)\right) = p(1-p)$ $\quad I_G(p) = 2\,Var\left(\mathcal{B}(p)\right)$

Example: Iris Dataset

Figure: Iris: setosa, versiocolor, virginica

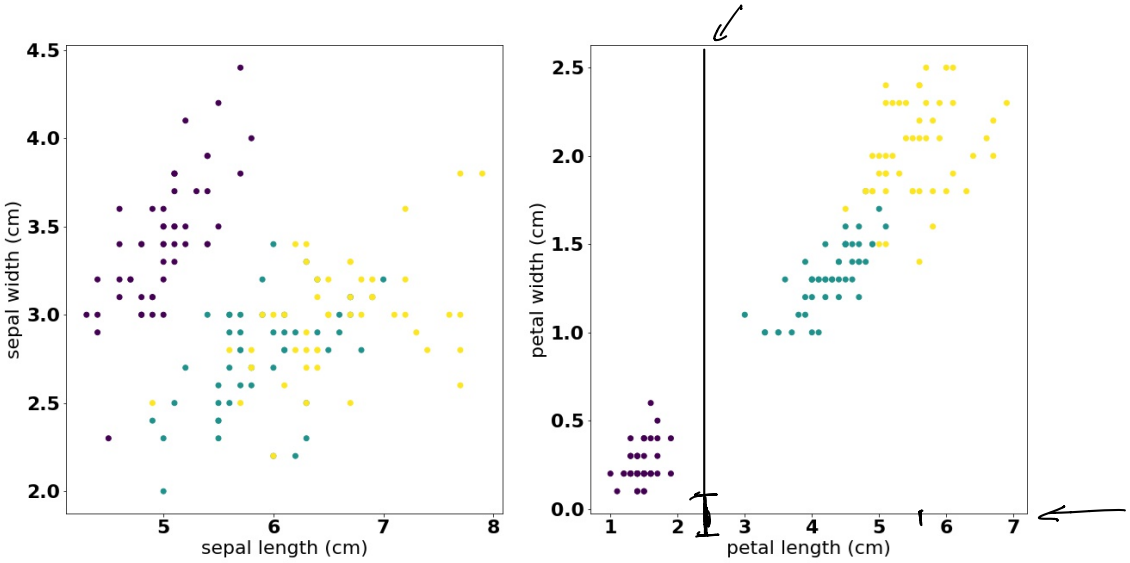
One of the most widely used toy dataset in classification:

- 3 classes : *['setosa', 'versicolor', 'virginica']*
- 50 points per class.
- 4 features: *['sepal length', 'sepal width', 'petal length', 'petal width']*



Only 2 cuts: very good accuracy.

Exercise: Guess Classification tree for Iris Dataset



cut is always a straight line

In pratice : Scikit Learn

Universal Python library for Machine Learning:

- Very easy to use
- Very well documented
- Open Source

`https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html`

Example: Iris Dataset

What do we need to specify ?

Step 1

Step 1 :: specify

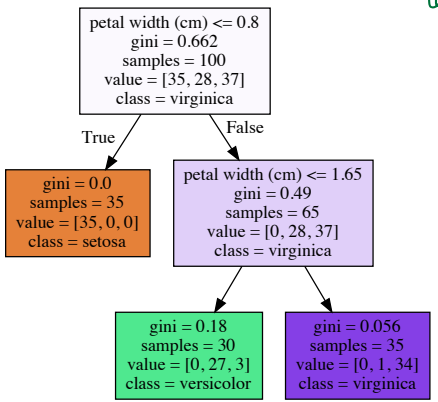
* impurity criterion : Gini is default
* stopping criterion : * tree_depth = 2

Fit model: X_{train}, Y_{train}

Step 2: clf.fit(X_{train}, Y_{train}) → learns the tree

```python
from sklearn.datasets import load_iris
from sklearn.model_selection import cross_val_score
from sklearn.tree import DecisionTreeClassifier, plot_tree
from sklearn.model_selection import train_test_split

# Choose the Learning algorithm
clf = DecisionTreeClassifier(max_depth = 2,
                             random_state=0)

#Load the dataset
iris = load_iris()
X_train, X_test, y_train, y_test = train_test_split(
    iris.data, iris.target, test_size=0.33, random_state=43)

#Check accuracy
cross_val_score(clf, iris.data, iris.target, cv=10)

# Fit the model
clf.fit(X_train,y_train)

# Plot tree
plot_tree(clf, feature_names = fn,
                class_names=cn,
                filled = True)
plt.show()
```

Output:



Example:

```python
# Check
X_test[0,:], iris.target_names[y_test[0]]
```

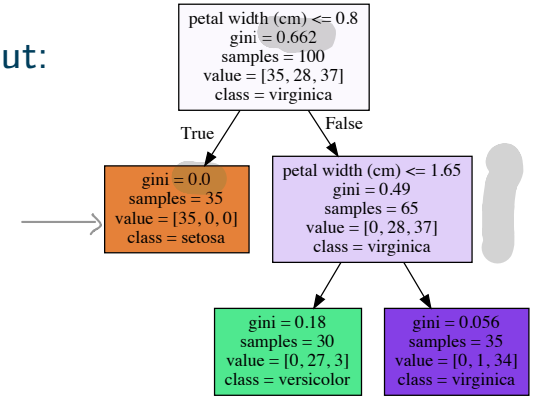
Returns:

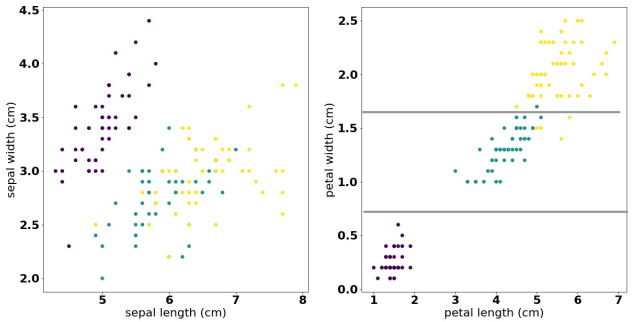
(array([4.8, 3.1, 1.6, 0.2]), 'setosa')

Code: https://colab.research.google.com/drive/1dXYIjacNAeASgl54vIWyWjMQlfgigSVA?usp=sharing#scrollTo=VeJHkJd7RsDw

Example: Iris Dataset

Output:





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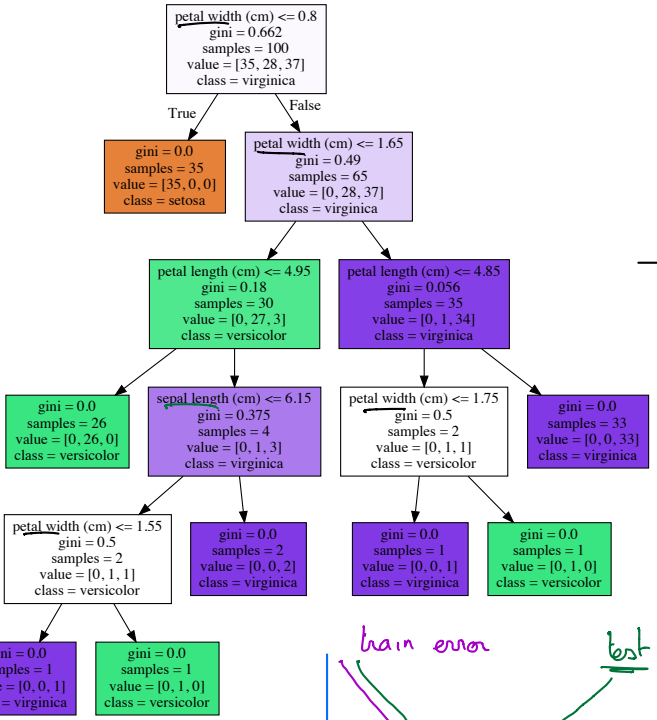
Code: https://colab.research.google.com/drive/1dXYIjacNAeASgl54vIWyWjMQlfgigSVA?usp=sharing#scrollTo=VeJHkJd7RsDw

What if I use a deeper tree ? Or if I do not specify the depth in the model definition ?

Deeper trees

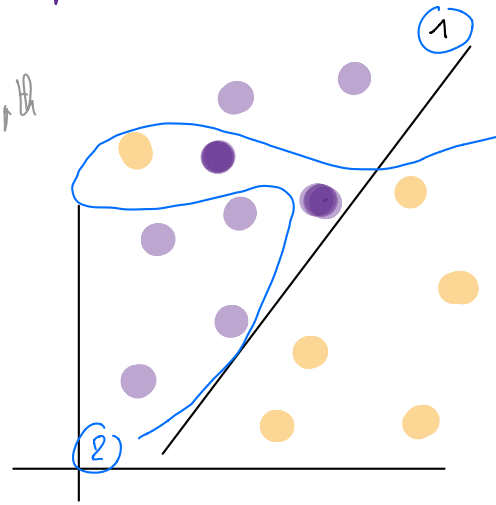
```
# Choose the Learning algorithm
clf = DecisionTreeClassifier(random_state=0)
```

defining model : no max-depth



Overfitting:

* very good accuracy on training
* degraded acc on test

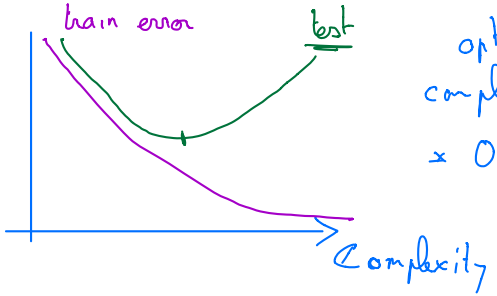


option 1 is simple

* but 1 error train set
* less errors on test set

option 2 is more complex

* 0 error train set



- When does the algorithm stop then ?
- What do you think about it ?

Stopping / Pruning

Trees that achieve perfect classification may suffer from over-fitting. (see example in the lab)

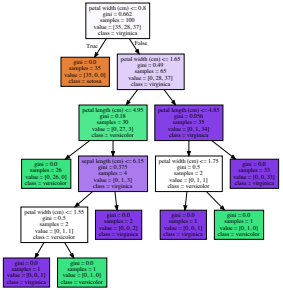
To avoid this problem, we can reduce the complexity of the trees:

1. Stopping rules
   - Set a minimum number of samples inside each leaf.
   - Set a maximum depth.
2. Pruning
   - Reduced error pruning.
   - Cost complexity pruning.

easier in practice

Pruning : example of Cost complexity pruning.

We create a sequence of Trees by changing one subtree at each step into a leaf, until we get only the root: the subtree is chosen to minimize the error made.[1] Then the test error is evaluated along the sequence, to choose the optimal pruning.



[1] *more details here*

Cart: pros and cons

11h15.

Pros:

- Simple to understand, interprete, visualize
- Implicitly perform features/variable selection
- can handle both categorical and numerical data
- little effort for data preparation
- Non linear relationships do not affect performance
- Can work with large number of observations.

Cart is always using only one feature

Cons:

1. Can create over-complex trees: overfitting
2. Unstability: small variations of data can generate completely different trees
3. Cannot guarantee global optimal tree iterative construction
4. Biased if some classes dominate

Solution : Using Random Forests !

Outline

Random Forests

To put it in simple words: « random forests builds multiple decision trees and merges them together to get a more accurate and stable predictions ».
↳key idea: create variable trees + aggregate them

How to create variability ?

- Instead of the most important features, search the best feature among a random subset (ntry). → sklearn
- Work on subsets of data (bootstrap=True).
- More https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestRegressor.html

X_{train}, Y_{train} : to built tree n°i, you use a random subset i X_{train} ; Y_{train}

1st. step : defining the model. all hyperparam. / options

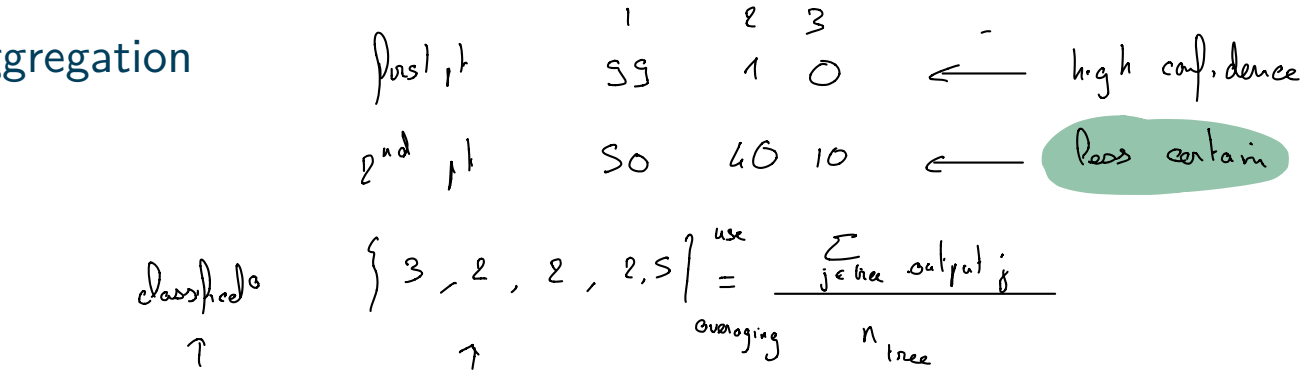
2nd step : fitting model.

```
# Creating and fitting a Random Forest
from sklearn.ensemble import RandomForestClassifier

plt.figure(figsize=(20,10))
clf = RandomForestClassifier(n_estimators = 100,
                             max_depth=3, bootstrap = True,
                             random_state=0)

clf.fit(X_train,y_train)
```

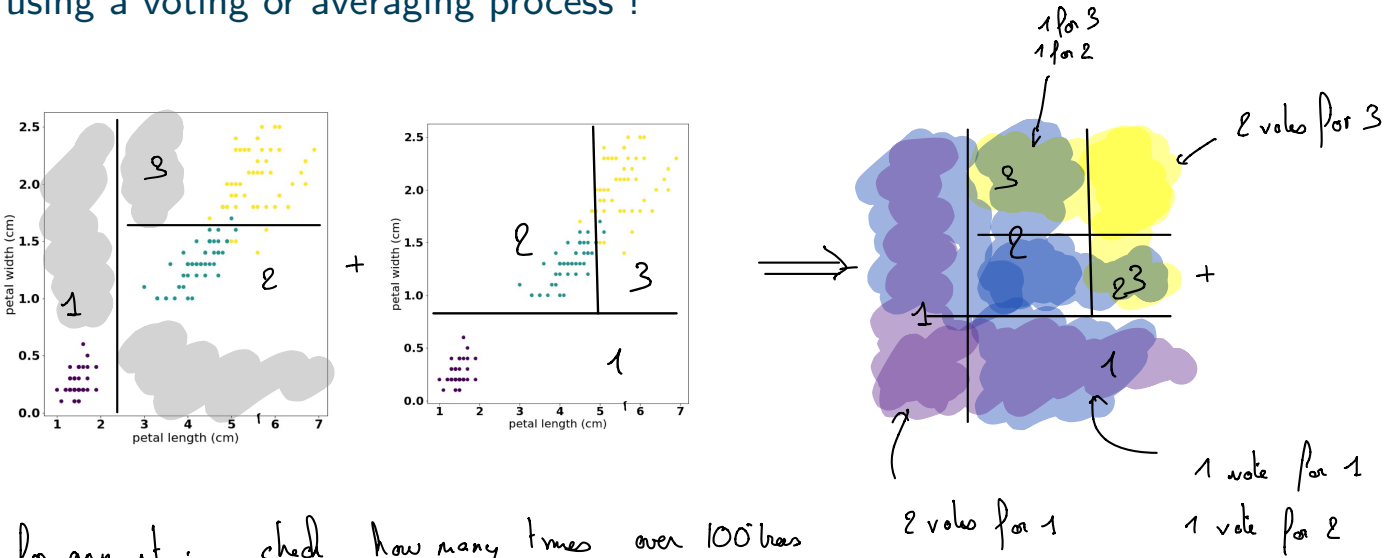
100 trees in it
all trees have depth 3
use bootstrap.

How to aggregate ? How to interpret a Random Forest ?

Aggregation



We using a voting or averaging process !



For any pt : check how many times over 100 trees it is placed in each category ?

60 times cat 1 | 20 times 2 | 20 times cat 3 ⟹ final classif 1

Feature importance

- how much tree nodes using a particular feature reduce impurity along the trees.
- suggests feature selection rule: drop out features with low importance to avoid overfitting.
- Attribute **feature_importance_** in RandomForestRegressor of Sklearn.

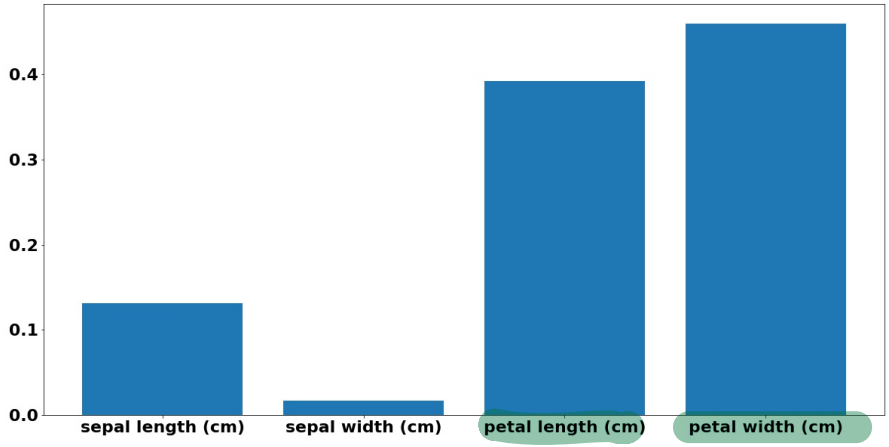


Figure: Feature importane output for a Random Forest Classifier in Python

Comparison with decision trees

arguments / hyperparams
* specific to the forest: * number trees
* randomness split (max features, bootstrap)
* related to each tree: * max_depth * min_sample_leaf

RF: already existed for DT

Cons:

- Less interpretable ✓
- Slower to run ✓

Pros:

- Better in higher dimension ✓
- More stable outputs ✓
- Feature selection ✓

Improving predictions - more arguments.

1. **n_estimators** : number of trees in the forest
   - improves prediction / stability
   - slows down the algorithm
2. **max_features** : maximum number of features considered to split a node
3. **min_sample_leaf** : minimum number of samples that should remain in a leaf node.

RF pros and cons

RF Pros:

1. works for classification and regression
2. default hyperparameters often produce reasonable prediction -> easy to use.
3. avoid overfitting if some good trees in the forest and easy feature selection -> high dimensional pb.
4. hard to beat in performance.

RF Cons:

1. Fast to train but slow to provide new predictions -> ineffective for « real-time predictions ».
2. Good for prediction but bad for description.

What about Regression ? ⟶ use MSE instead of Gini for each tree

⟶ use averaging instead of voting to aggregate the trees.

Questions?

Boosting

⊕ gain in accuracy / preci°

⊖ no distribut° possible of th workload.

Another import technique (very powerful !)

Main idea:

- Give more importance to difficult point iteratively
- Incrementally building an ensemble by training each new instance to emphasize the training instances previously mis-modeled.

Example: AdaBoost

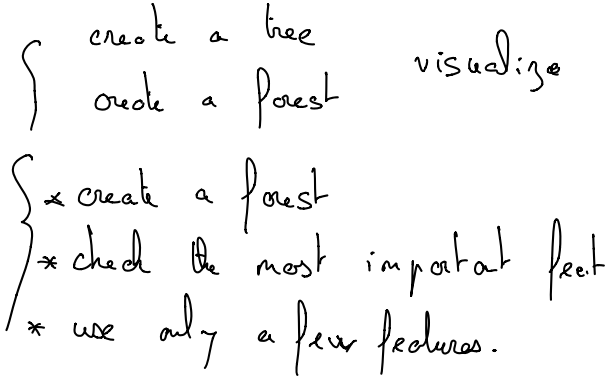
See: `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.AdaBoostClassifier.html`

Conclusion

1. Trees are one of the simplest method (the most intuitive / human like)
2. Random Forests give excellent results in many applications.

Lab :

- Example on a synthetic dataset of time series.
- Application to inflation prediction in Brazil.



Meta Lab:

- Python.
- Colab: - need to connect to ggl account
  - save the nb at beg. & end.
-