ML, Decision Trees and Random Forests
Data science Certificate

Aymeric DIEULEVEUT

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Outline

A Reminder on Supervised Learning

- Observations: $(X_i)_{i=1,\dots n}$. Each X_i has d components.
- Outputs: $(Y_i)_{i=1,\dots n}$

3 Examples:

- Iris Dataset:
- MNIST:
- House price prediction

Example 1: House price Prediction - Regression

Goal: observe the features for a house, predict its price.

House price Prediction dataset $Y \in \mathbb{R}_+$

- Output : house value

  $\rightarrow Y \in \mathbb{R} \rightarrow$ *regression* task

- 1500 examples

  $\rightarrow n = 1500$

- 81 features: Construction year, Neighborhood, Surface, Floor, Balcony: both quantitative and qualitative, some ordinal variables.

  $\rightarrow X \in \mathbb{R}^{81}$.

SML goal.

* Learn the link $X \rightarrow Y$.
* From n examples
* Predict well on a new X_{test}

$X_{\text{Aymeric\_flat}} = (1970, 13^e, 60, 4, \text{Yes}, \dots)$

Example 2: Iris Dataset - Classification

Figure: Iris: setosa, versiocolor, virginica

Goal: identify flower species based on petal/sepal characteristics.

Iris Dataset:

- 3 classes : *['setosa', 'versicolor', 'virginica']*

  $\rightarrow$ $Y \in \{0, 1, 2\}$ encoding each class.

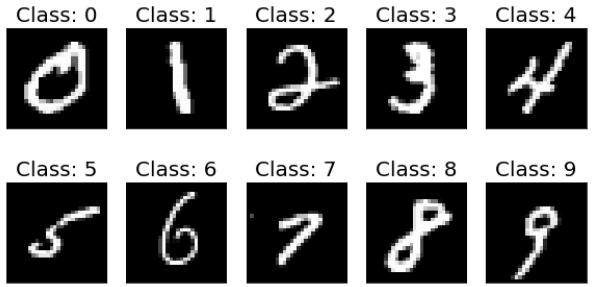
- 50 points per class

  $\rightarrow$ $n = 150$

- 4 features: *['sepal length', 'sepal width', 'petal length', 'petal width']*

  $X \in \mathbb{R}^4$, $\rightarrow$ $d = 4$

Example: MNIST Dataset



Goal: recognize an object on an image, e.g., a handwritten digit on its image.

Digit recognition from an image:

- 10 classes :

  $Y \in \{0, 1, 2, \ldots, 9\}$

- 60k images, (50k train, 10k test), balanced

  $n = 60000$

- Observation: pixels: 28*28 pixels per image (gray-scale).

  $X \in \mathbb{R}^{784}$, $d = 784$ features.

Summary of those three datasets

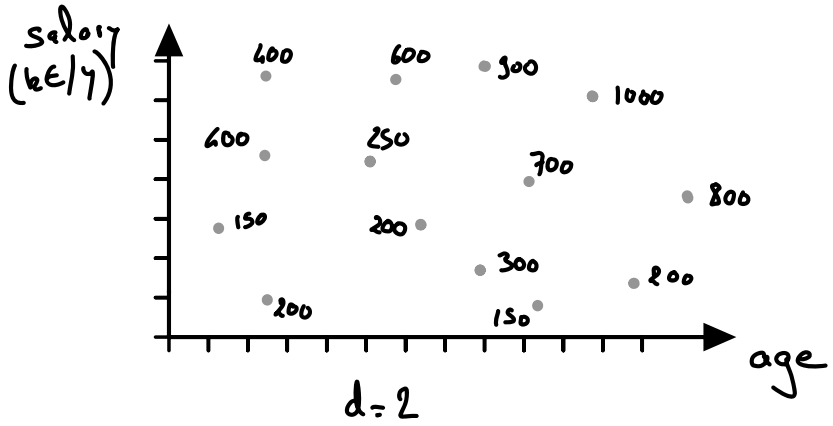
	Iris	MNIST	House price prediction
Number of examples n	150	60k	1500
Number of the features d	4	784	81
Type of the features	numerical values	numerical	categorical numerical ordinal (quantitative)
Space $\mathcal{Y}$	$\{0, 1, 2\}$ V, Vi, Se	$\{0, \dots 9\}$	$\mathbb{R}$
Task	C	C	R

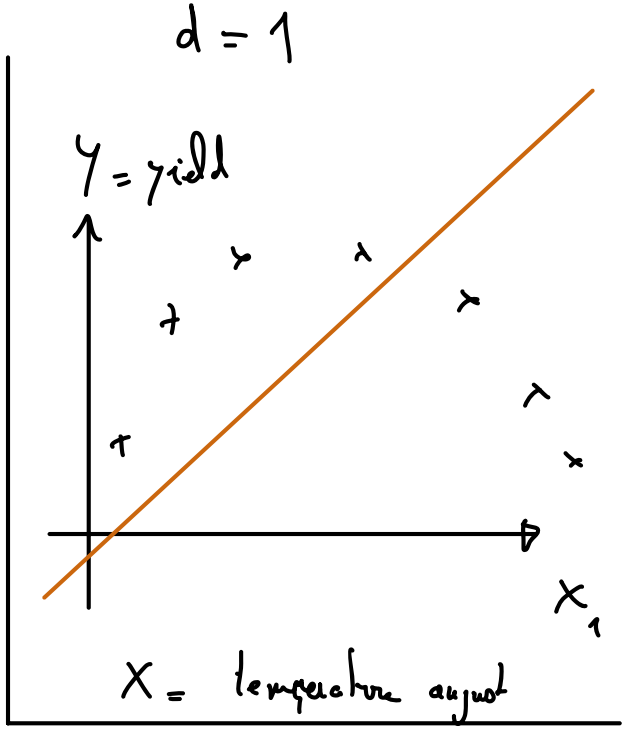
categorical → encoding.

Toy datasets

- In regression:

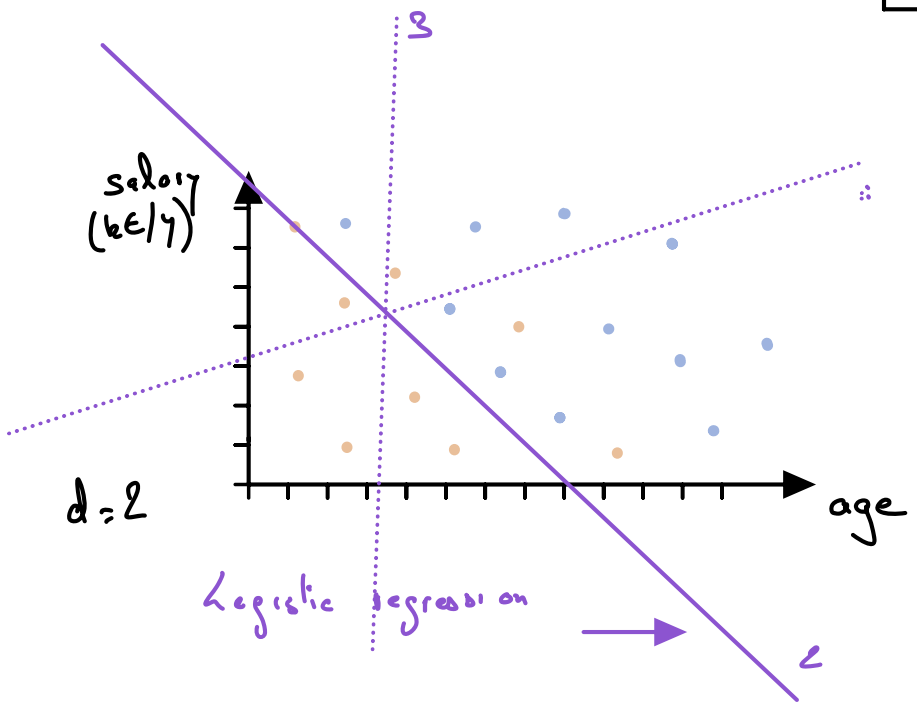
$X = (\text{age}, \text{salary})$





- In classification:

$X = (\text{age}, \text{salary})$

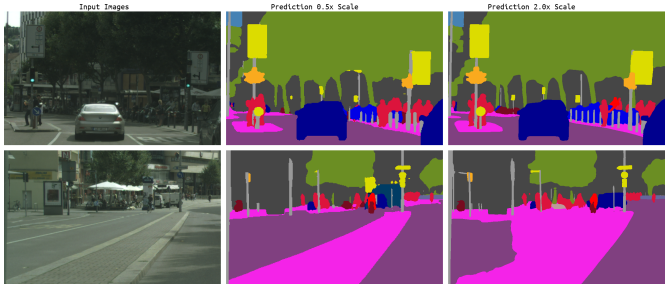


y

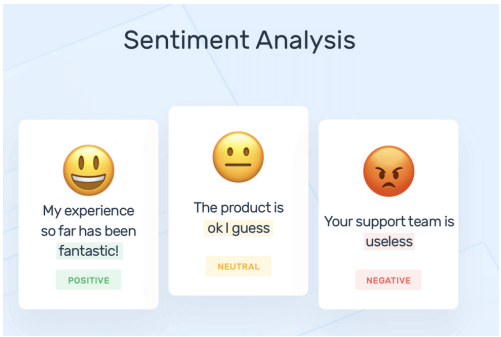
- rents his house
- owns his house

More examples

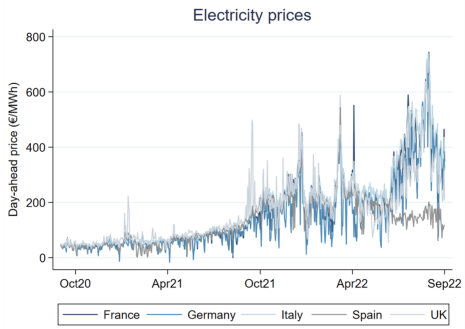
Spam detection



Semantic image segmentation



Sentiment classification

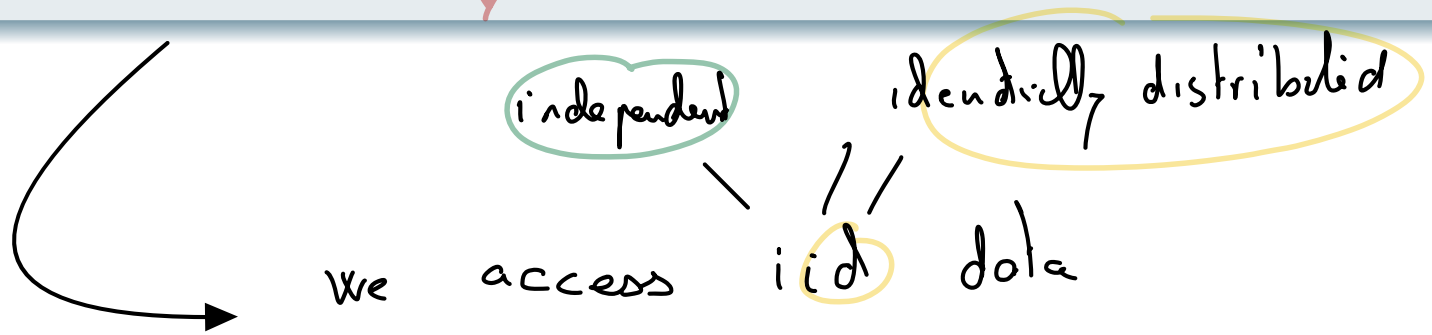


Electricity price forecasting

Supervised Learning

Supervised Learning

- Attributes / features / characteristics / input:
$$X \in \mathcal{X} = \mathbb{R}^d$$
- Output / Responses / label :
  - $Y \in \{-1, 1\}$ - binary classification,
  - $Y \in \{0, 1, 2, \ldots, K-1\}$ - multi-class classification,
  - $Y \in \mathbb{R}$ - regression.
- Phenomenon distribution $(X, Y) \sim \mathbb{P}$.



Critical assumption in ML: we learn to predict on a distrib°

Supervised Learning

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  - $Y \in \{-1, 1\}$ - binary classification,
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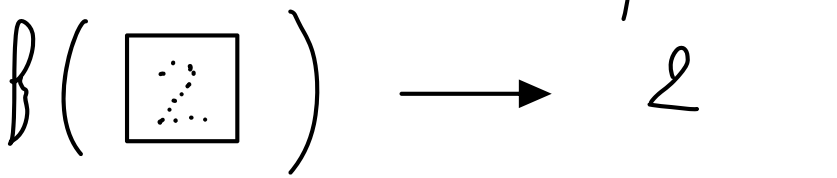
  - $Y \in \mathbb{R}$ - regression.
- Phenomenon distribution $(X, Y) \sim \mathbb{P}$.

- A classifier or predictor is a measurable function $g : \mathcal{X} \to \mathcal{Y}$.

How to **quantify the quality** of a predictor?



$\rightarrow$ introduce a risk function.

Loss function, Generalization Risk and data-dependent predictors

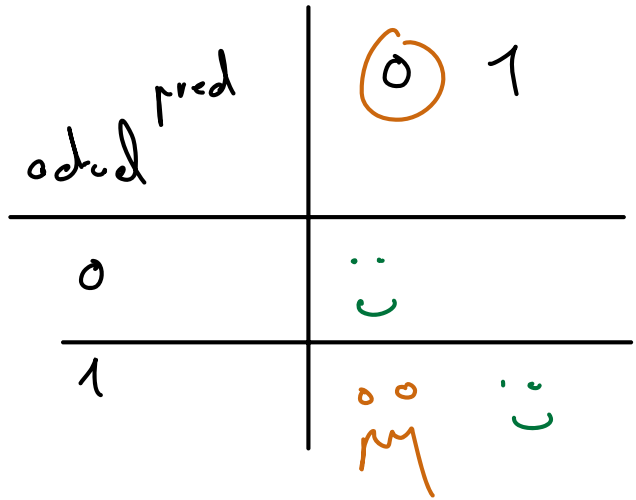
Loss Function

output predict

- Loss function: $\ell(y, g(x))$ quantifies the quality of the prediction $g(x)$ of y, e.g.:
  - 0-1 Loss (classification): $\ell(y, g(x)) = 1y \neq g(x), \quad y \in \mathcal{Y} = \{-1, 1\}$
  - Quadratic Loss (regression): $\ell(y, g(x)) = (y - g(x))^2, \ y \in \mathbb{R}$

choice of loss : complicated

* bycicle example



* what do we want ?

alignment

Loss function, Generalization Risk and data-dependent predictors

Loss Function

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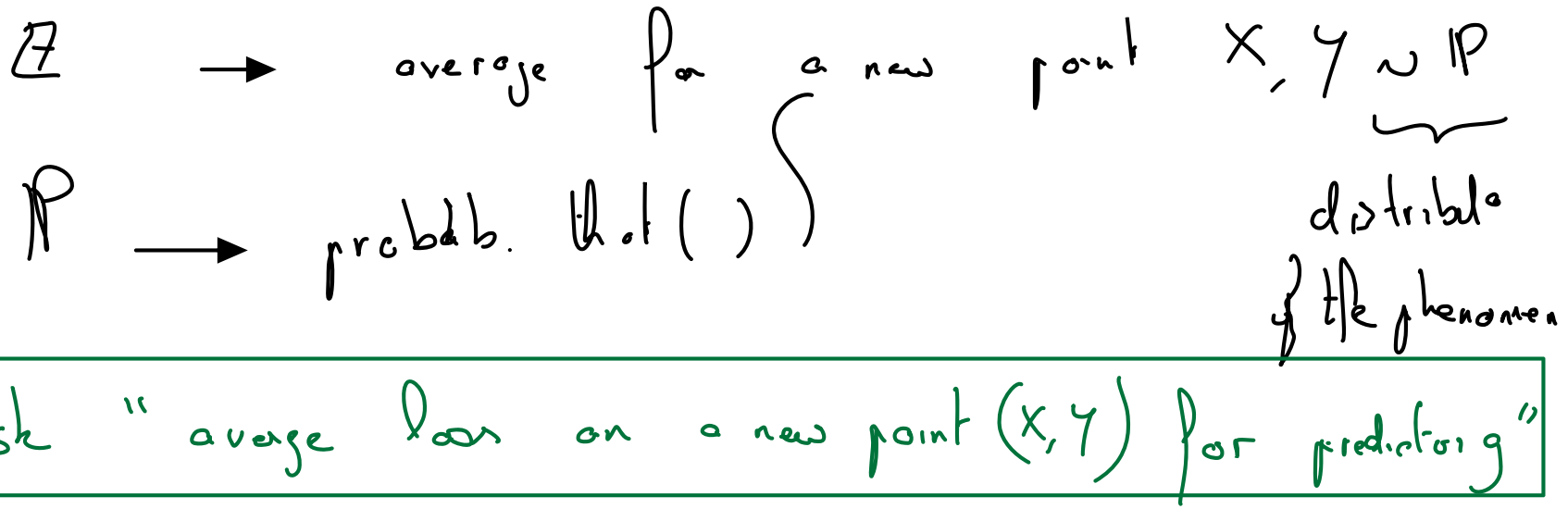
  - Quadratic Loss (regression): $\ell(y, g(x)) = \|y - g(x)\|^2$, $y \in \mathbb{R}^d$

Risk of a Decision Rule = average loss

- Risk: $R(g) = \mathbb{E}[\ell(Y, g(x))] = \int \ell(y, g(x)) d\mathbb{P}(x, y)$, e.g.:
  - 0-1 Risk (classification): $R(g) = \mathbb{P}(Y \neq g(x))$
  - Quadratic Risk (regression): $R(g) = \mathbb{E}[|Y - g(x)|^2]$

$\mapsto$ R is also referred to as *Generalization* risk, or *True* risk.



Loss function, Generalization Risk and data-dependent predictors

Loss Function

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$\mapsto$ R is also referred to as *Generalization* risk, or *True* risk.

⚠ The distribution $\mathbb{P}$ is unknown.

Data-dependent predictors

- Training set: $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\} \quad (i.i.d. \sim \mathbb{P})$
- Goal: build a data dependent predictor / classifier $\widehat{g}_n$ based on the training data
- That has a minimal generalization risk $R(\widehat{g}_n)$.

$R(\widehat{g}_n)$ = average loss on a "new point" $(X, Y) \sim \mathbb{P}$, independent from D_n

$\leftrightarrow$ Our goal is to predict well on inputs/outputs pairs that **we have not seen in the dataset**, i.e. *generalize* well.

THM 1.

Supervised Learning: Summary

2 levels of understanding:

1. * generic pipeline (algos are Black box)
2. * opening the black box for each algo.

Supervised Learning: Framework Summary

- Training set: $D_n = \{(x_1, Y_1), \ldots, (x_n, Y_n)\} \quad (i.i.d. \sim \mathbb{P})$
- Decision rule (classifier, predictor): $g : \mathcal{X} \to \mathcal{Y}$ ~~measurable~~
- Loss: $\ell(Y, g(x))$
- Risk: $R(g) = \mathbb{E}[\ell(Y, g(x))] = \int \ell(y, x) d\mathbb{P}(x, y)$

Numerous methods:

1. In **regression**:
   - linear, polynomial, (kernel regression)
   - (regularized methods (Lasso, Ridge))
2. In **classification**:
   - Logistic regression
   - SVM → also linear classifiers
3. For **both**
   - Nearest neighbors
   - Random forests
   - Neural networks
   - etc.

Supervised

unsupervised

Reinforcement

today !

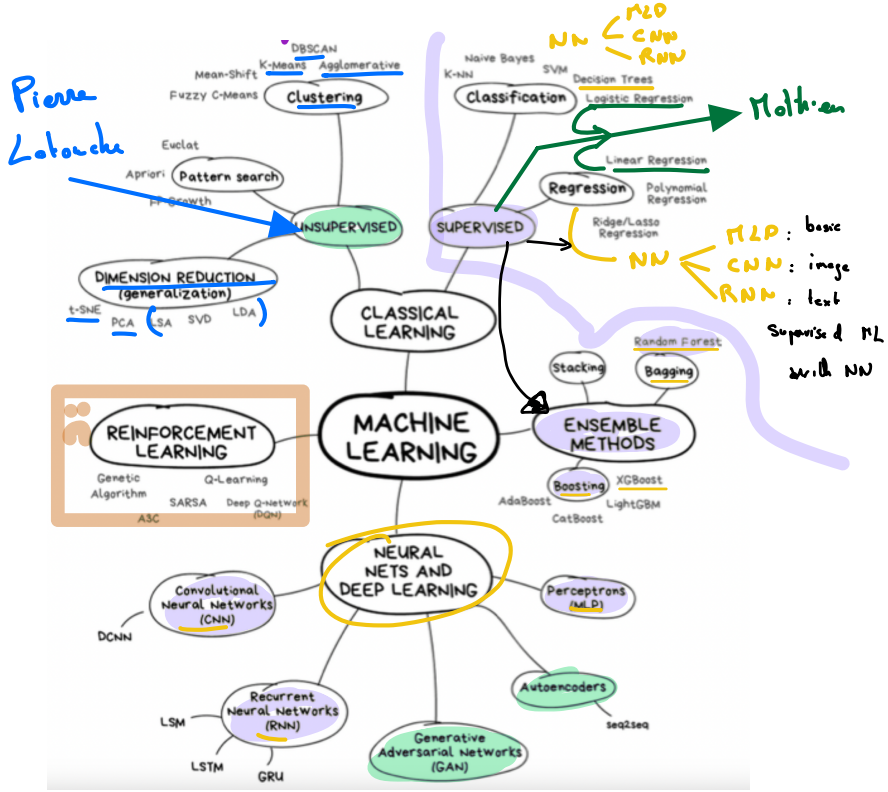


Figure:

2 levels of understanding:

1. * generic pipeline (algos are Black box)
2. * opening the black box for each algo.

(1) → how to do ML without knowing exactly what algo do?

Learn parameters: automatically | computed / optimized | by the computer to perform well on the Train set

user does nothing

Digression : knowing methods (obj 2)
enables to know which ones (ops)

* Speed
* Interpretability
* Performance

The ordering S / I / P depends on the task.

High freq trading S - P

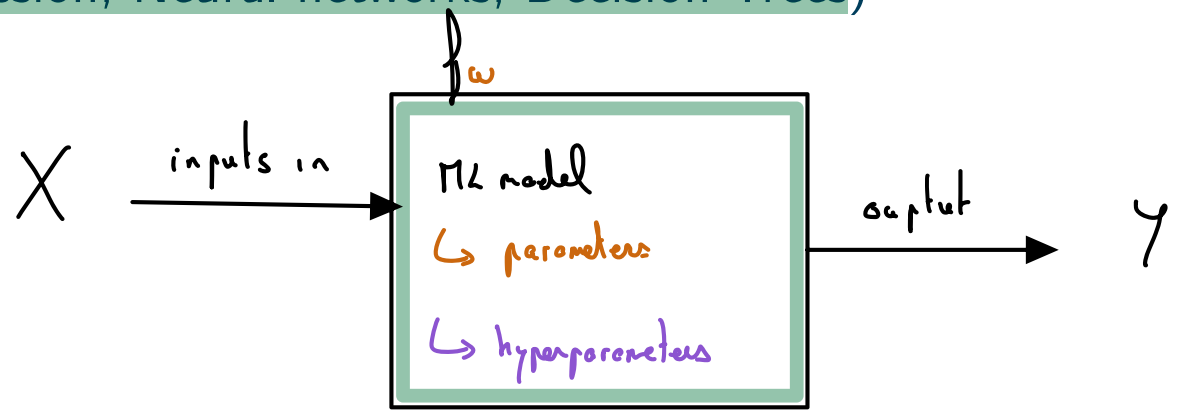
Treatment prediction : P - I

credit assignt (: regulated env) P - I

Learning Pipeline

1. **Training**

   Learn the dependency between input and output. Each model (LR, Logistic regression, Neural networks, Decision Trees)



parameters :

Linear regression

House price prediction

$X = (\text{surf}, \text{surf bdc})$

$f_\omega(X) = X_1 \omega_1 + X_2 \omega_2$

$10\,k€/m^2$ si $3€/m^2$

f_ω : insist on parameter dependence

ω : parameters

Training phase: give Train dataset $\mathcal{D}_{Tr}$

" Fitting phase "

$\longrightarrow \min_\omega$ risk f_ω on $\mathcal{D}_{Tr}$

computer $\longrightarrow$ finds the "best/good" parameters ω w.r.t. Train set

hyperparameters are chosen by the user :

* nb of trees in forest
* architecture
* model type

Solution :

* expert knowledge
* "cross validated"

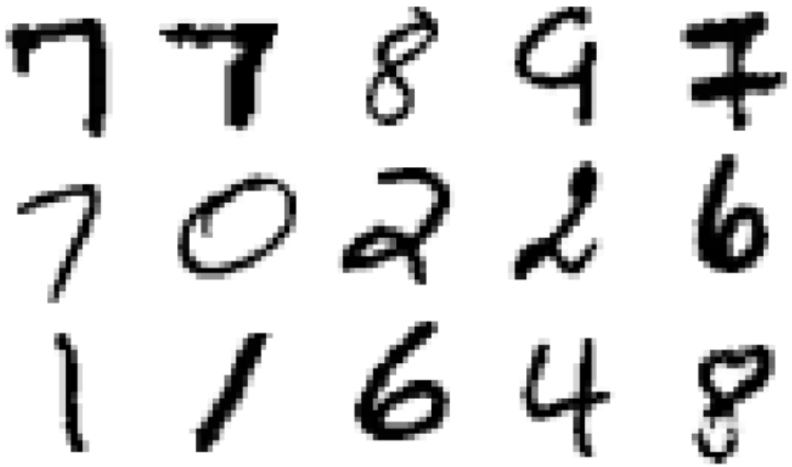
" try many pick the best

Fitting a method

Demo url (Lab): https://colab.research.google.com/github/adieulev/Certificate-DS-2023/blob/main/Labs/MWE_ML_init_student_version.ipynb

```python
import numpy as np
from sklearn.datasets import fetch_openml
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import accuracy_score

# Fetching the MNIST dataset
mnist = fetch_openml('mnist_784', version=1)
X, y = mnist["data"], mnist["target"]

# Setting aside 10% of the data
X_sample, _, y_sample, _ = train_test_split(X, y, test_size=0.9, random_state=42)

X_train, X_test, y_train, y_test = train_test_split(X_sample, y_sample, test_size=0.2, random_state=42)

# Scaling the data
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train.astype(np.float64))
X_test_scaled = scaler.transform(X_test.astype(np.float64))

import warnings
warnings.filterwarnings('ignore')
```

Figure: Importing data



Fitting

Fitting a method

Entrée [37]:
```
from sklearn.tree import DecisionTreeClassifier

dt_clf = DecisionTreeClassifier(                    )
dt_clf.fit(X_train_scaled, y_train)
```
0s
105

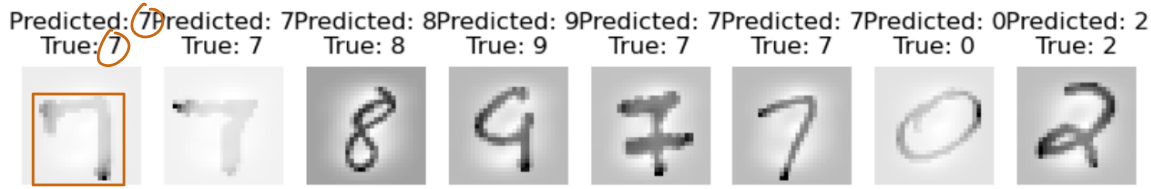
choose hyperparameters !!

here : none !

Out[37]:
```
DecisionTreeClassifier(random_state=42)
```

"train on train data" = "fit" = "learn w"

Entrée [38]:
```
predictions = dt_clf.predict(X_train_scaled[:16])
fig, axes = plt.subplots(1, 8, figsize=(10, 2))  # Adjust the figure size as needed
for i, ax in enumerate(axes):
    ax.imshow(X_train_scaled[i].reshape(28, 28), cmap=plt.cm.gray_r, interpolation='nearest')
    ax.set_title(f"Predicted: {predictions[i]}\nTrue: {y_train.iloc[i]}")
    ax.axis('off')
plt.show()
```



Entrée [39]:
```
from sklearn.ensemble import RandomForestClassifier

rf_clf = RandomForestClassifier(n_estimators=10,random_state=42)
rf_clf.fit(X_train_scaled, y_train)
```
0s
1005

fitted w

hyperparam : nb of trees.

Out[39]:
```
RandomForestClassifier(n_estimators=10, random_state=42)
```

Entrée [40]:
```
from sklearn.linear_model import LogisticRegression

log_reg = LogisticRegression(multi_class="multinomial", solver="lbfgs", max_iter=100, random_state=42)
log_reg.fit(X_train_scaled, y_train)
```

loss

solver

fitted w

Out[40]:
```
LogisticRegression(multi_class='multinomial', random_state=42)
```

Figure: Fitting 3 methods and predicting

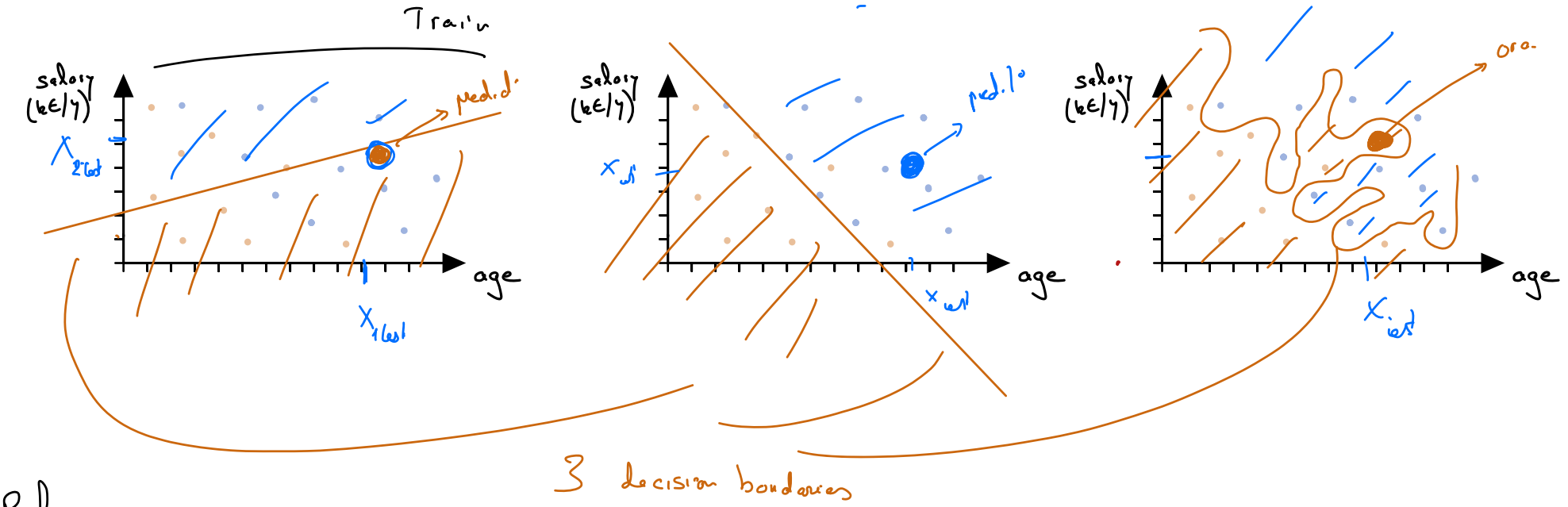
What is true about SML

1. Supervised Machine Learning does not have inputs ✗
2. Supervised Machine Learning can be combined with unsupervised in some contexts ✓
3. Supervised Machine Learning does not have outputs ✗
4. The goal is to predict well on new unseen points ✓ ✓
5. It is necessary to perform well on the train set for that ✓ (99%)
   - most of the time, yes
   - S' It is sufficient to perform well on the train ✗
6. The goal is to predict well on the train points ✗
7. The balance interpretability/speed/performance depends on the method ✓
8. I assume my training data to be representative (iid) of a phenomenon with distribution P ✓

Caveat: Overfitting - Toy datasets

⚠ The perfomance on the training set may not reflect the ability to predict on a future point !!

💡 Our Goal is to perform well on unseen outputs!!



3 decision boundaries

Perf on					
Train	bad (underfitting)	ok +	3 mistakes	:v	0 mistakes
Test	bad	good - good fit		:(bof	overfitting

💡 Need to focus on validation/test performance

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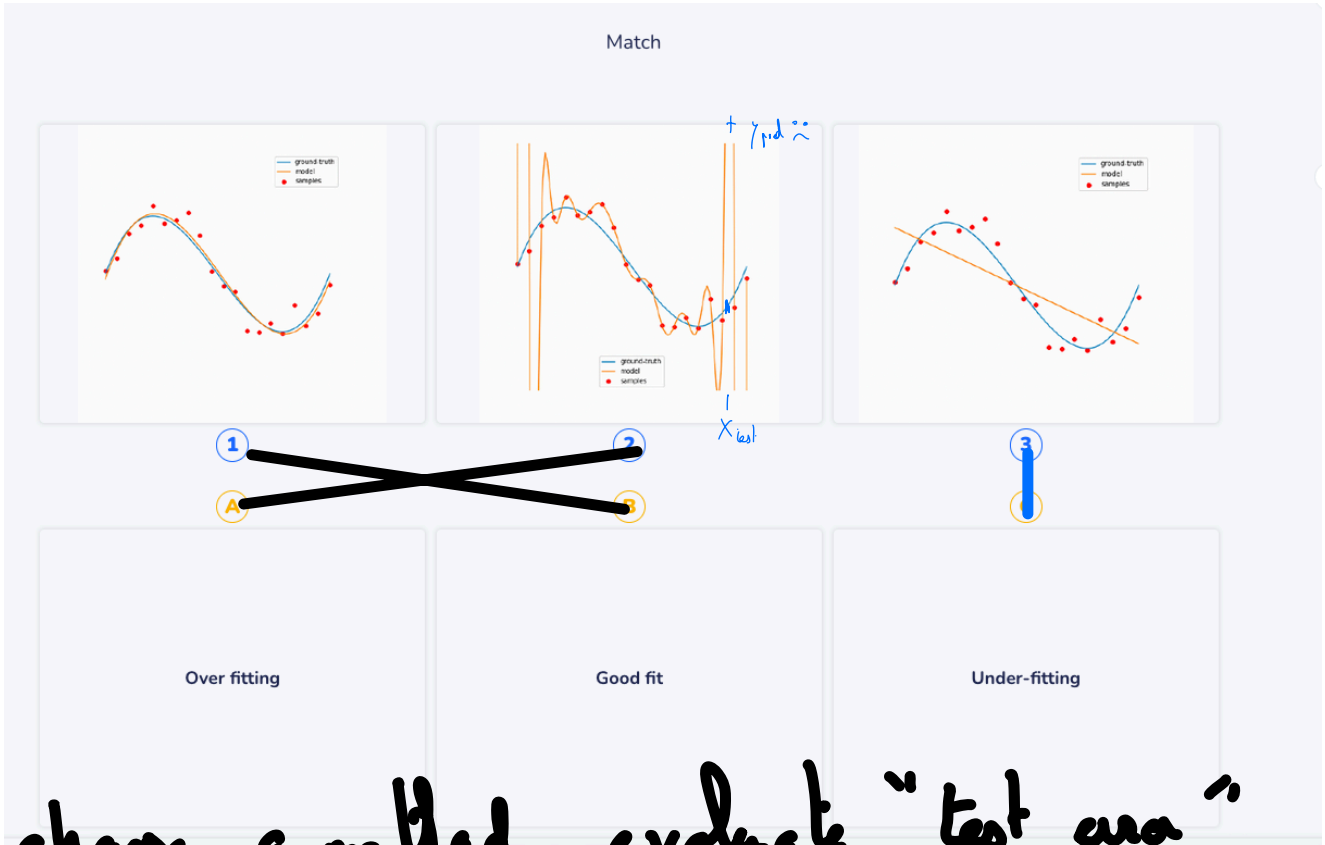


overfitting

My perfomance on the test is much worse than on the train

to choose a method, evaluate "test error" approximate

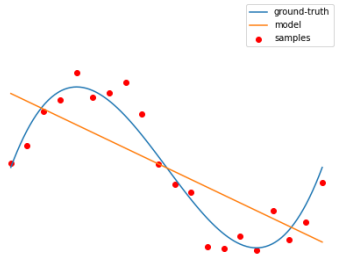
Underfitting : I do not even learn on the train

💡 Need to focus on validation/test performance

Underfitting and Overfitting depending on the choice of $\mathcal{C}$

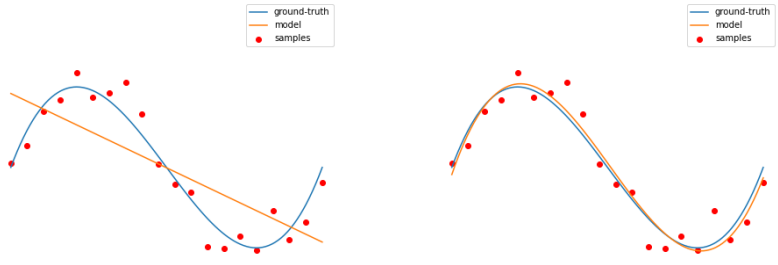
$\mathcal{C} =$
$\hat{R}_n(\theta_n^*)$
$R(\theta_n^*)$
Problem
Dim. of Θ

Underfitting and Overfitting depending on the choice of $\mathcal{C}$



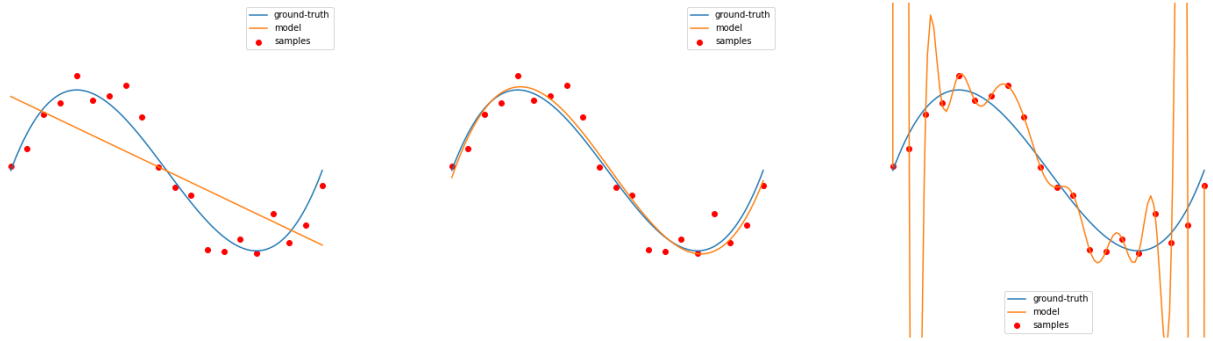
$\mathcal{C} =$	Affine functions
$\hat{R}_n(\theta_n^*)$	high
$R(\theta_n^*)$	high
Problem	Underfitting
Dim. of Θ	2

Underfitting and Overfitting depending on the choice of $\mathcal{C}$



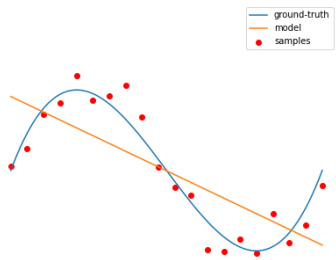
$\mathcal{C} =$	Affine functions	$\mathbb{R}_3[X]$
$\hat{R}_n(\theta_n^*)$	high	low
$R(\theta_n^*)$	high	low
Problem	Underfitting	All good
Dim. of Θ	2	4

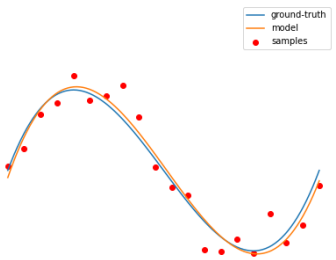
Underfitting and Overfitting depending on the choice of $\mathcal{C}$

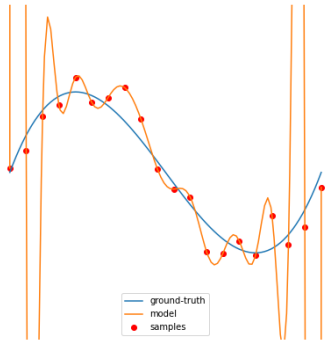


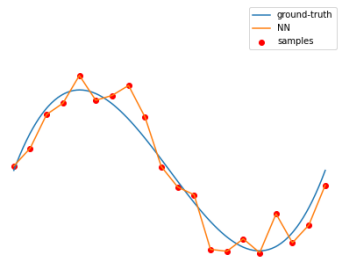
$\mathcal{C} =$	Affine functions	$\mathbb{R}_3[X]$	$\mathbb{R}_{19}[X]$
$\hat{R}_n(\theta_n^*)$	high	low	zero
$R(\theta_n^*)$	high	low	high
Problem	Underfitting	All good	Overfitting
Dim. of Θ	2	4	20

Underfitting and Overfitting depending on the choice of $\mathcal{C}$









$\mathcal{C} =$	Affine functions	$\mathbb{R}_3[X]$	$\mathbb{R}_{19}[X]$	FCNN
$\hat{R}_n(\theta_n^*)$	high	low	zero	zero
$R(\theta_n^*)$	high	low	high	mid low
Problem	Underfitting	All good	Overfitting	
Dim. of Θ	2	4	20	17375

Demo Colab

Learning Pipeline

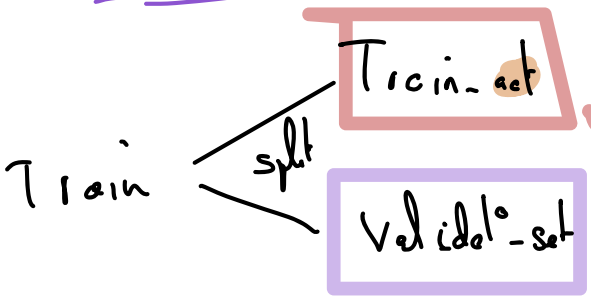
Split data as Tr + Test

1. **Training phase**

For all hyperparameters / models :

Learn ω for a given model & hyperparameters on Tr_{in}

Fit (learned by computer) (chosen / proposed by the user)



→ output $\hat{f}_{\hat{\omega}}$

2. **Validation phase** → compare methods in a fair way

→ evaluate the prediction $\hat{f}_{\hat{\omega}}$ on Validat° set

→ fair estimat° of the performance (for all method & hyperparam)

3. **Test phase** Test →

Final evaluat° of the model.

4. **Deployment** if test error is satisfying, move to deployment

One algorithm to rule SML: Cross validation

Enables to select the best method within mutliple methods

Entrée [7]:

```
models = {
    "Decision Tree": DecisionTreeClassifier(random_state=42),
    "Random Forest": RandomForestClassifier(n_estimators=10,random_state=42),
    "Logistic Regression": LogisticRegression(multi_class="multinomial", solver="lbfgs", max_iter=100, random_st
    "MLP Classifier": MLPClassifier(random_state=42),
    "SVM": SVC()
}
```

Entrée [12]:

```
cv_results = {}

for name, model in models.items():
    kfold = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)
    cv_score = cross_val_score(model, X_train, y_train, cv=kfold, scoring="accuracy")
    cv_results[name] = cv_score
    print(f"{name}: Mean CV accuracy={np.mean(cv_score)}, Std Deviation={np.std(cv_score)}")
```

```
Decision Tree: Mean CV accuracy=0.77125, Std Deviation=0.013163512495701512
Random Forest: Mean CV accuracy=0.8826785714285714, Std Deviation=0.008957097288560329
Logistic Regression: Mean CV accuracy=0.875, Std Deviation=0.007804204779790029
MLP Classifier: Mean CV accuracy=0.8842857142857143, Std Deviation=0.0031237242293813998
SVM: Mean CV accuracy=0.9505357142857143, Std Deviation=0.005463235193135154
```

Entrée [18]:

```
# Convert results to DataFrame for better visualization
results_df = pd.DataFrame(cv_results)
results_df
```

Out[18]:

	Decision Tree	Random Forest	Logistic Regression	MLP Classifier	SVM
0	0.775893	0.885714	0.880357	0.885714	0.953571
1	0.752679	0.875000	0.866071	0.882143	0.942857
2	0.776786	0.898214	0.883929	0.885714	0.958929
3	0.790179	0.881250	0.865179	0.888393	0.950000
4	0.760714	0.873214	0.879464	0.879464	0.947321

Entrée [17]:

```
# Descriptive statistics can also be helpful
results_df.describe()
```

Out[17]:

	Decision Tree	Random Forest	Logistic Regression	MLP Classifier	SVM
count	5.000000	5.000000	5.000000	5.000000	5.000000
mean	0.771250	0.882679	0.875000	0.884286	0.950536
std	0.014717	0.010014	0.008725	0.003492	0.006108
min	0.752679	0.873214	0.865179	0.879464	0.942857
25%	0.760714	0.875000	0.866071	0.882143	0.947321
50%	0.775893	0.881250	0.879464	0.885714	0.950000
75%	0.776786	0.885714	0.880357	0.885714	0.953571
max	0.790179	0.898214	0.883929	0.888393	0.958929

Figure: Cross Validation

One algorithm to rule SML: Cross validation

Enables to select the best hyperparameters for a given methods

Leveraging grid search CV

Entrée [ ]:

```python
from sklearn.model_selection import GridSearchCV

# Example for SVM
param_grid = {
    'C': [1, 10, 100],
    'gamma': [0.001, 0.01, 0.1],
}
grid_search = GridSearchCV(SVC(), param_grid, cv=3, verbose=2)
grid_search.fit(X_train_scaled[:10000], y_train[:10000])  # Reduced data size for quicker execution

print("Best parameters:", grid_search.best_params_)
print("Best cross-validation accuracy:", grid_search.best_score_)
best_model = grid_search.best_estimator_
final_predictions = best_model.predict(X_test_scaled)
print("Test set accuracy:", accuracy_score(y_test, final_predictions))
```

Entrée [43]:

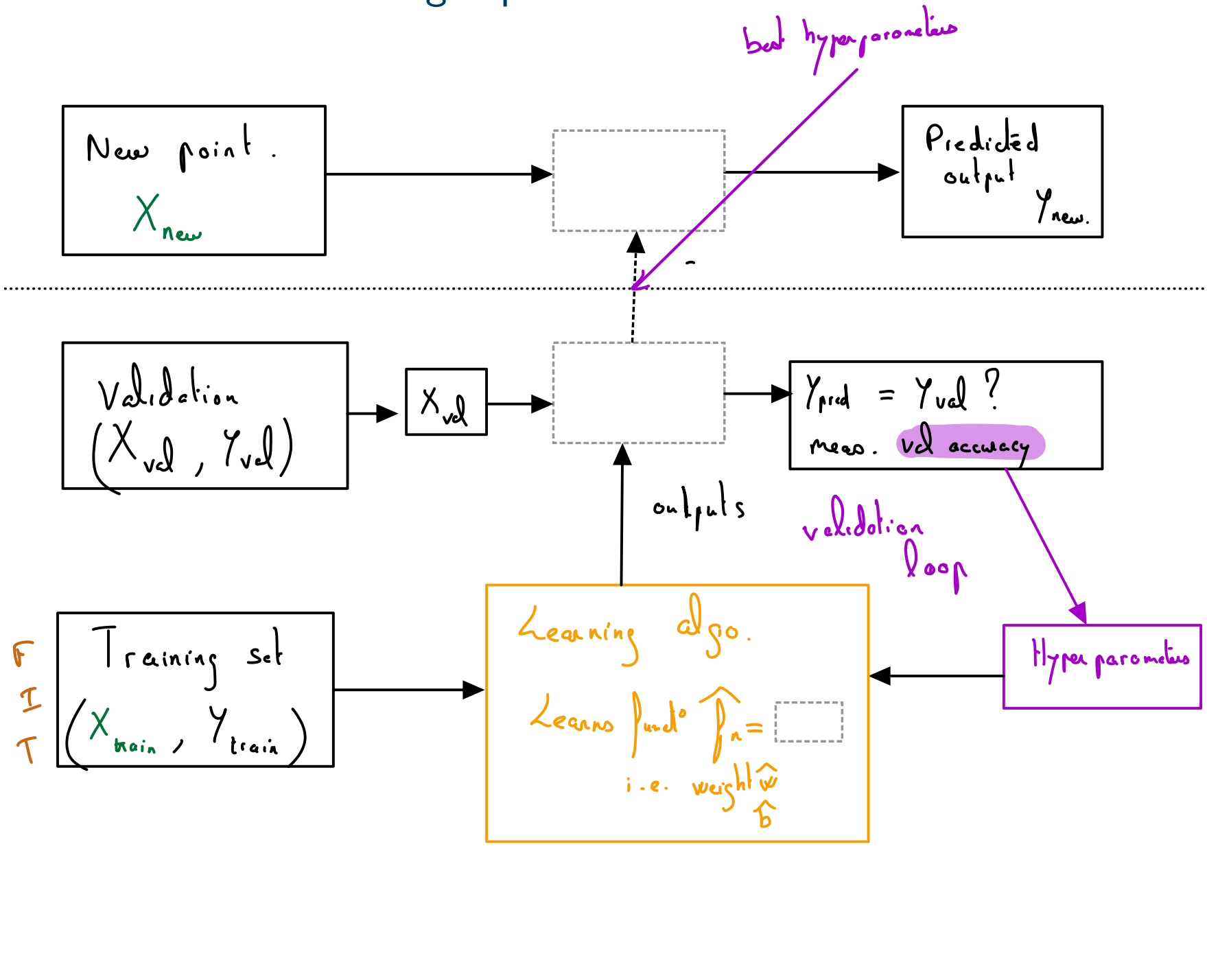
```python
pd.DataFrame(grid_search.cv_results_)
```

Out[43]:

	mean_fit_time	std_fit_time	mean_score_time	std_score_time	param_C	param_gamma	params	split0_test_score	split1_test_score	split2_test_score	mea
0	2.354261	0.049712	1.981289	0.027614	1	0.001	{'C': 1, 'gamma': 0.001}	0.918050	0.930370	0.927653	
1	7.614626	0.022478	2.995119	0.006781	1	0.01	{'C': 1, 'gamma': 0.01}	0.693626	0.718800	0.724009	
2	8.525636	0.034385	3.381043	0.004120	1	0.1	{'C': 1, 'gamma': 0.1}	0.175147	0.187467	0.181136	
3	1.957532	0.022052	1.767812	0.001655	10	0.001	{'C': 10, 'gamma': 0.001}	0.928227	0.933048	0.937835	
4	7.731749	0.122276	3.002695	0.004842	10	0.01	{'C': 10, 'gamma': 0.01}	0.708623	0.735404	0.746517	
5	8.540356	0.023448	3.378721	0.004322	10	0.1	{'C': 10, 'gamma': 0.1}	0.176219	0.187467	0.184887	
6	1.959067	0.025085	1.774580	0.014967	100	0.001	{'C': 100, 'gamma': 0.001}	0.928763	0.933048	0.937835	
7	7.861557	0.143017	3.017998	0.025798	100	0.01	{'C': 100, 'gamma': 0.01}	0.708623	0.735404	0.746517	
8	8.649604	0.021181	3.455342	0.009529	100	0.1	{'C': 100, 'gamma': 0.1}	0.176219	0.187467	0.184887	

Figure: Grid search CV

Supervised Machine Learning Pipeline



SML -Summary

1. Key concepts
   - Tasks
   - Methods
   - Overfitting and cross validation

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2. Black box solution:

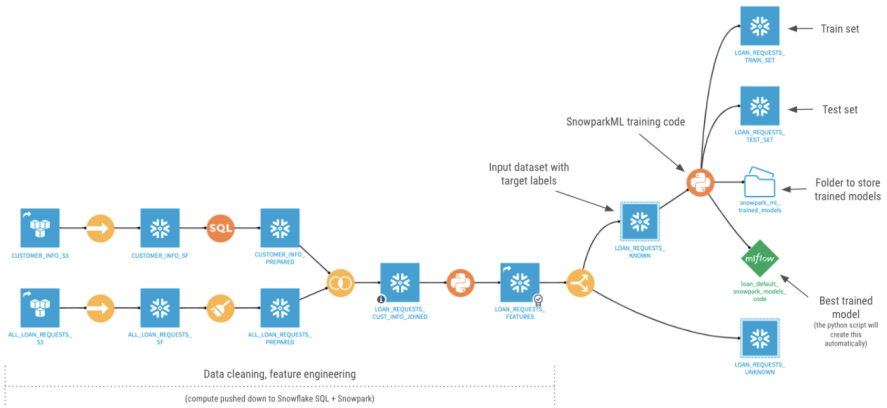

Figure: Dataiku

`https://blog.dataiku.com/training-ml-models-with-dataiku-and-snowpark-ml-a-code-approach`

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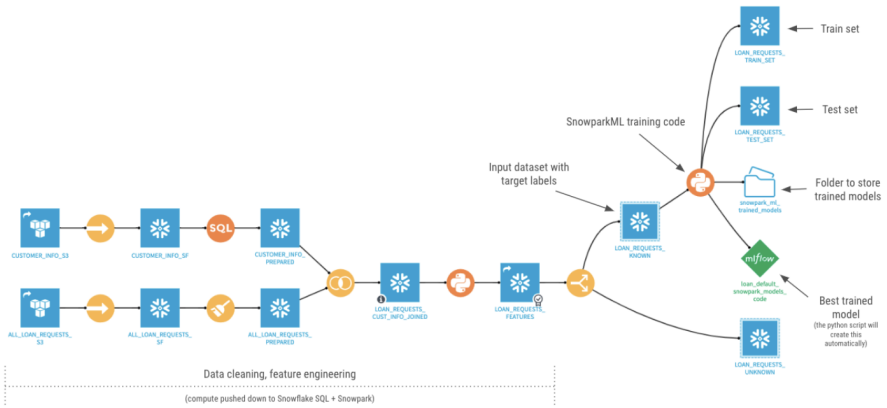

Figure: Dataiku

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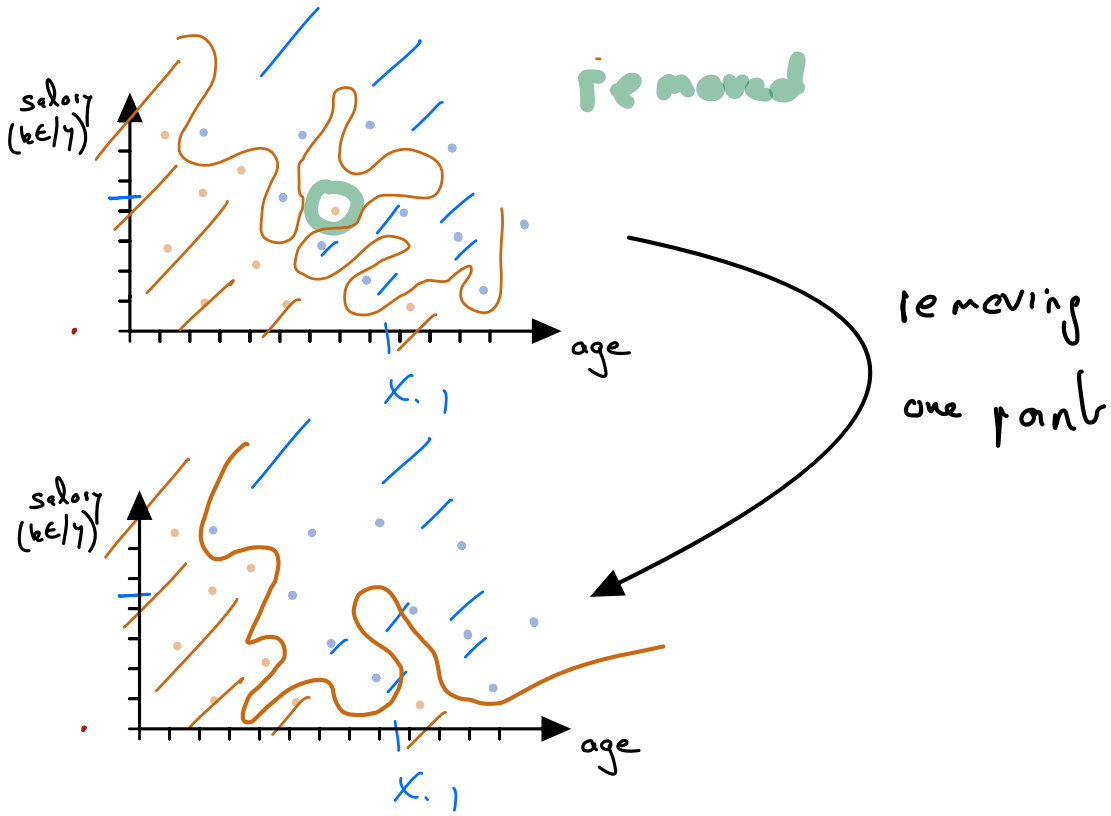
3. 💡 Our goal for today and tomorrow: **Opening the black box**
   → Understanding methods enables to better anticipate the best choice, limits, potential, etc.
   → Better choices for hyper-parameters to be chosen

Afternoon Woodop.

What is the problem of overfitting

1. I will have a bad error on the train set ✗
2. I will have a bad error on the test set ✓
3. My predictor may change a lot if I change the training set



What is the role of cross validation

1. Find the best model in terms of validation error ✓
2. Find the best parameters in terms of training error ✗ (although we do several fits with cv)
3. Find the best hyperparameters in terms of validation error ✓
4. Fit the model ✗ (")
5. Find the best parameters in terms of validation error ✗

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CV:

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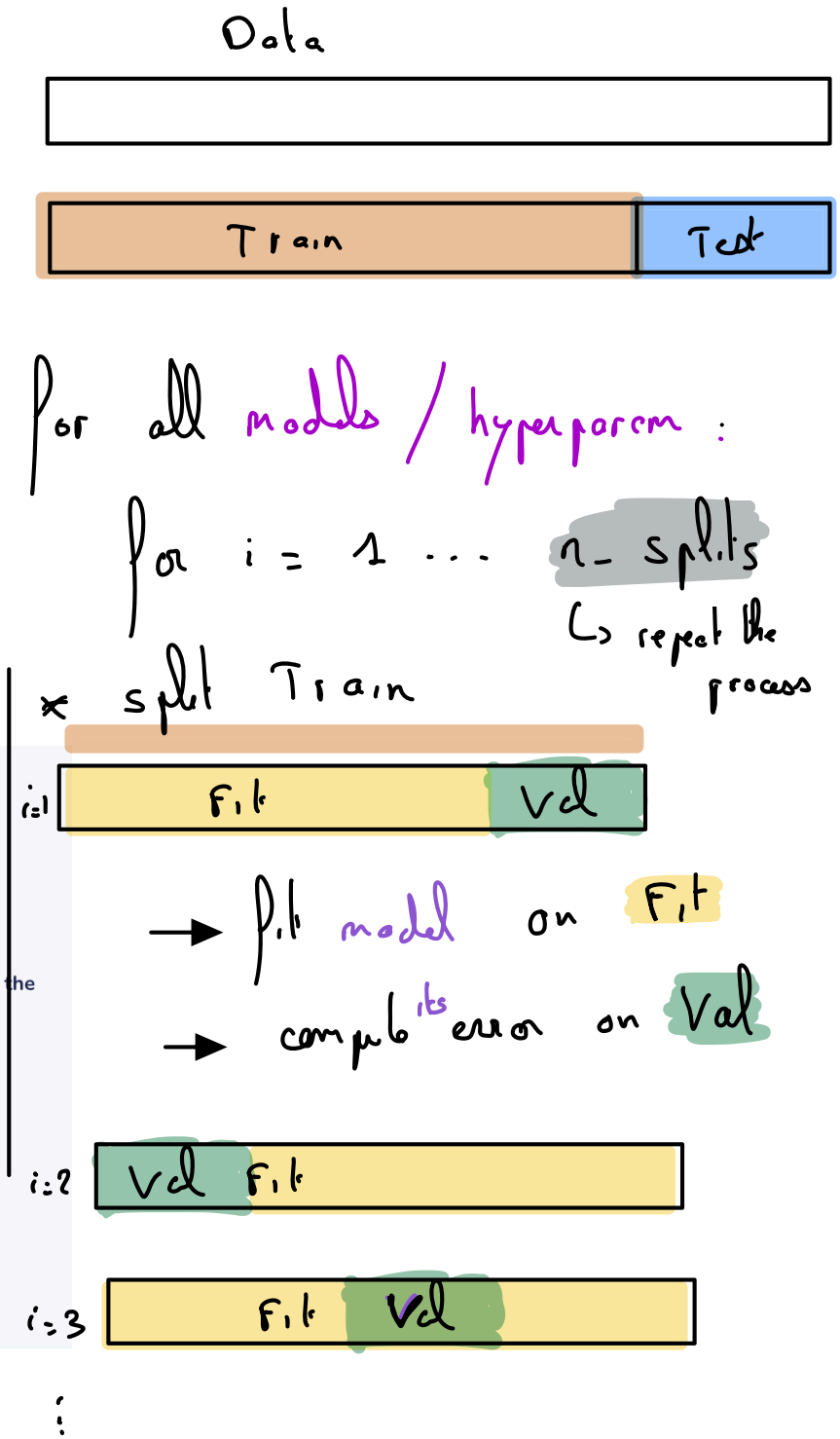
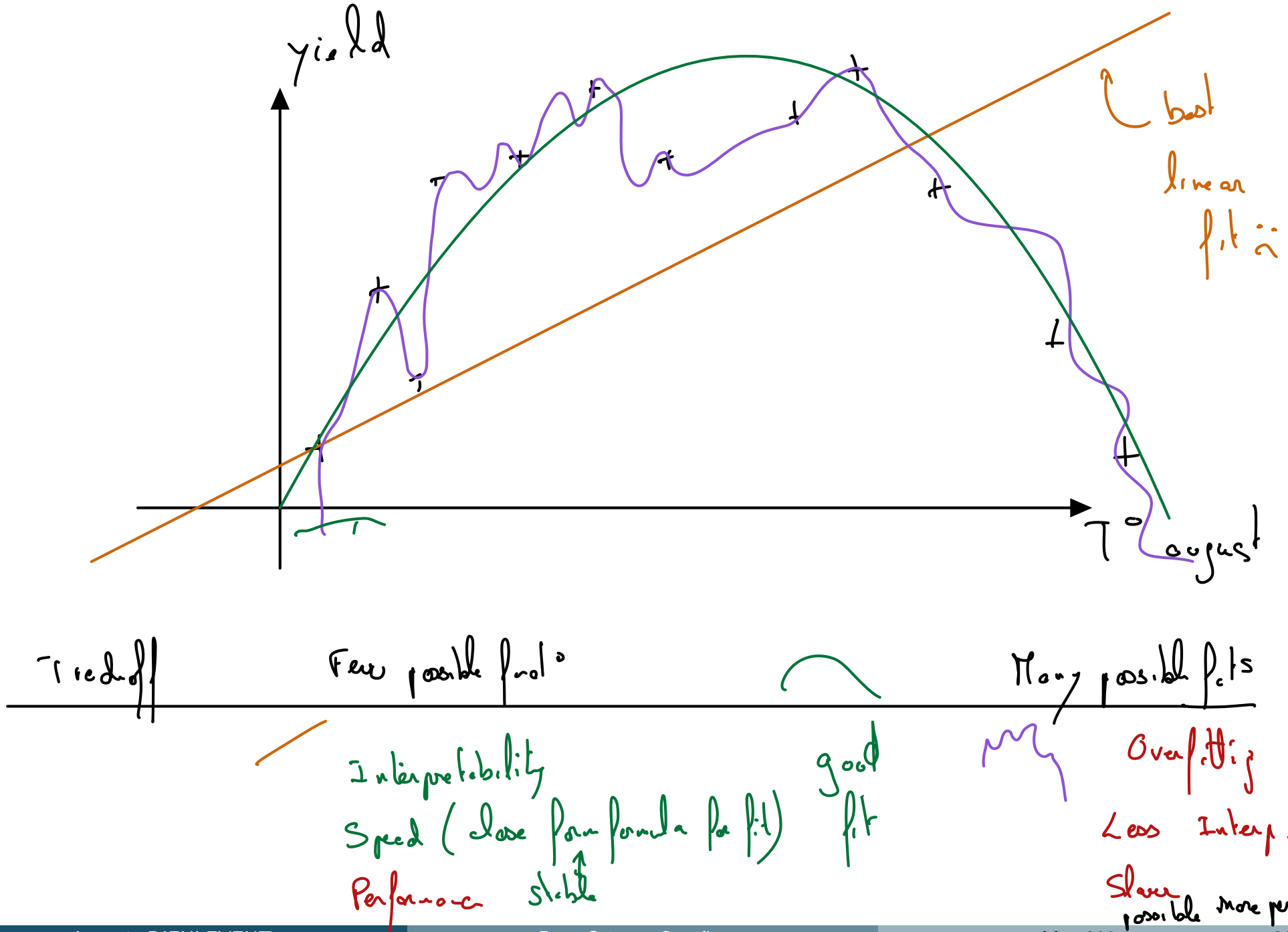
finding a fair estimate of the generalisation risk of the model

What does this code do

1. It enables to compare the five methods given above ✓
2. It computes Train score for each method
3. It computes Validation score for each method ✓
4. It computes 5 scores for each method, splitting the test data
   ↳ never used
5. It computes 5 scores for each method, splittin the train data
   as Cd, Fit ✓
6. The best method is SVM ✓
7. About 95% of the digits are well classified on the calibration set ✓
8. Random forest outperform Decision Trees
   88% vd. acc vs 77% vd acc
9. 25 fits were performed overall
   ✓ (expensive)
10. 5 fits were performed overall X



Reminder on Linear and Logistic regression - towards DT



Limits of Linear and logistic regression - towards DT

Outline

Decision Tree

Goals of Decision Trees

1. Supervised Learning: solve the classification or regression task
2. Provide some understanding: what on this example allows me to classify it? What are the important features ?
3. Go beyond linear functions $\longrightarrow$ allow complex dependencies.

Decision Tree

Goals of Decision Trees

1. Supervised Learning: solve the classification or regression task
2. Provide some understanding: what on this example allows me to classify it? What are the important features ?
3. Go beyond linear functions $\longrightarrow$ allow complex dependencies.

Two questions:

- How to train a decision tree? $\rightarrow$ **training phase (learning algorithm)**
- How to predict with a given decision tree? $\rightarrow$ **inference phase**

Inference Phase

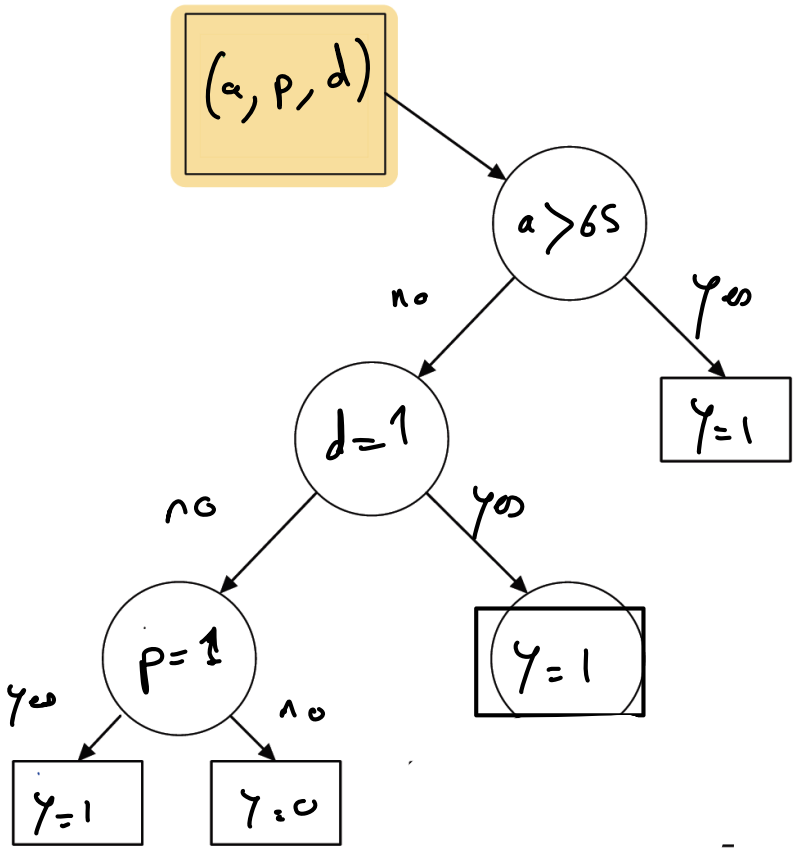
Can get Covid shot example

(age, precedit, doctor)

(a, p, d)

- Root = observation = input
- Nodes = tests

  → based on a single variable
- Branches = possible outcomes
- Leaves = final decision = output



Each node = 1 test = | 1 feature
1 threshold.

Training: how to build a tree.

fit

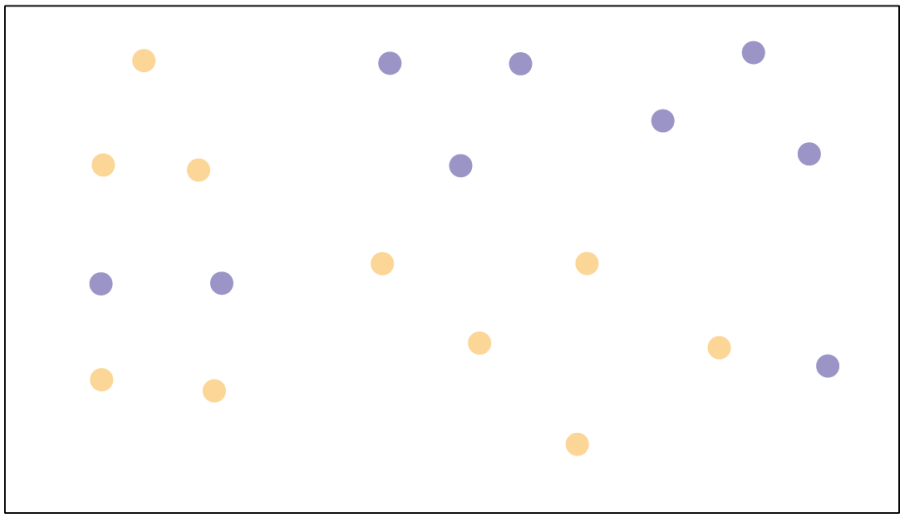
to a dataset $X_{[i,1]}, Y_{[i,t]}$

Key question !

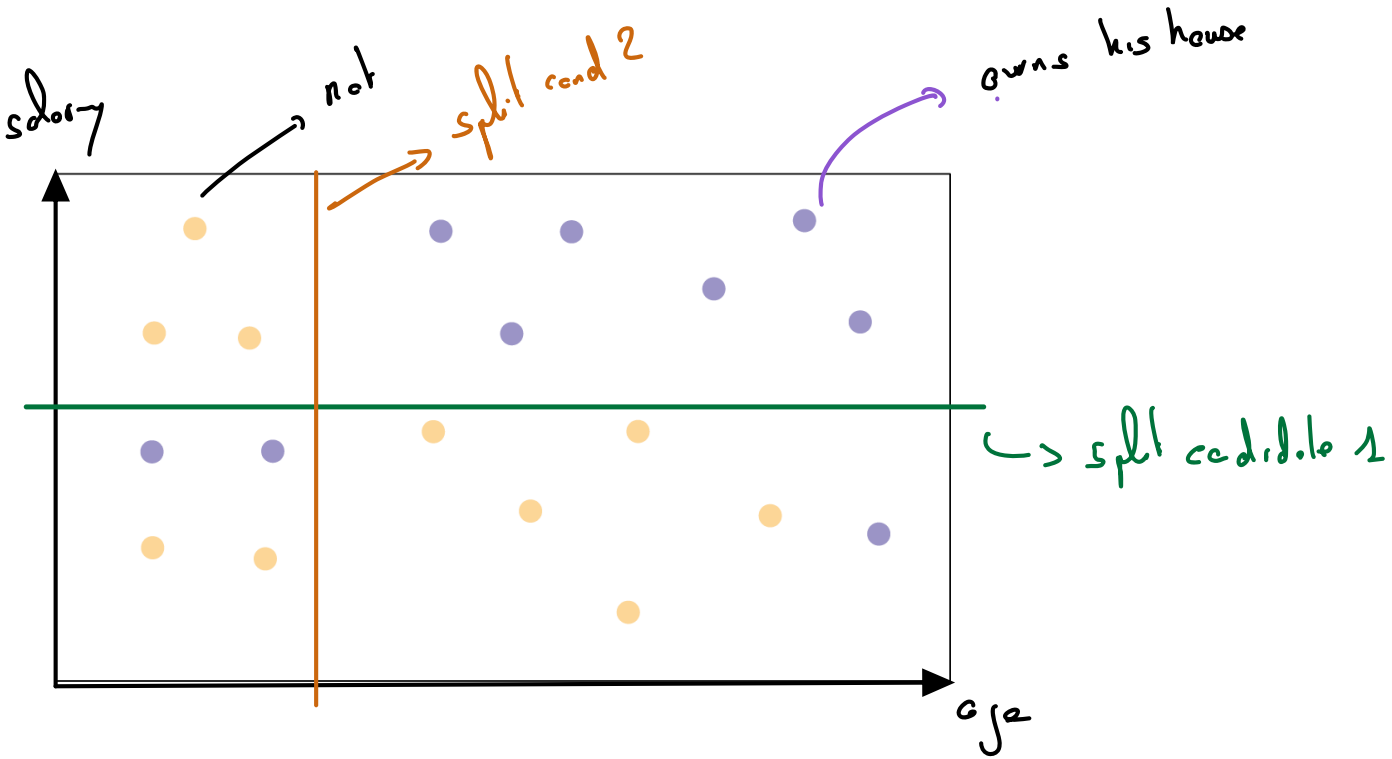
- What is a good tree?
- What do I need to choose?
- How to choose?

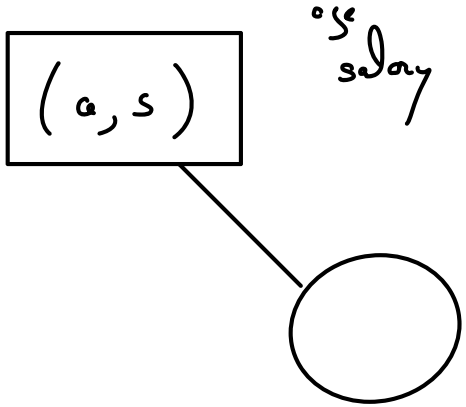
What do you think?

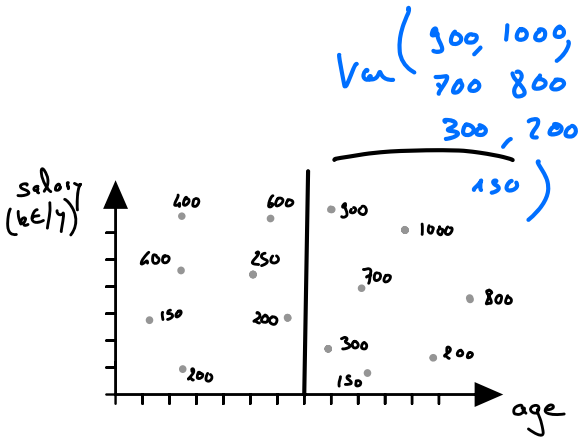
Building trees : CART



Building trees : CART



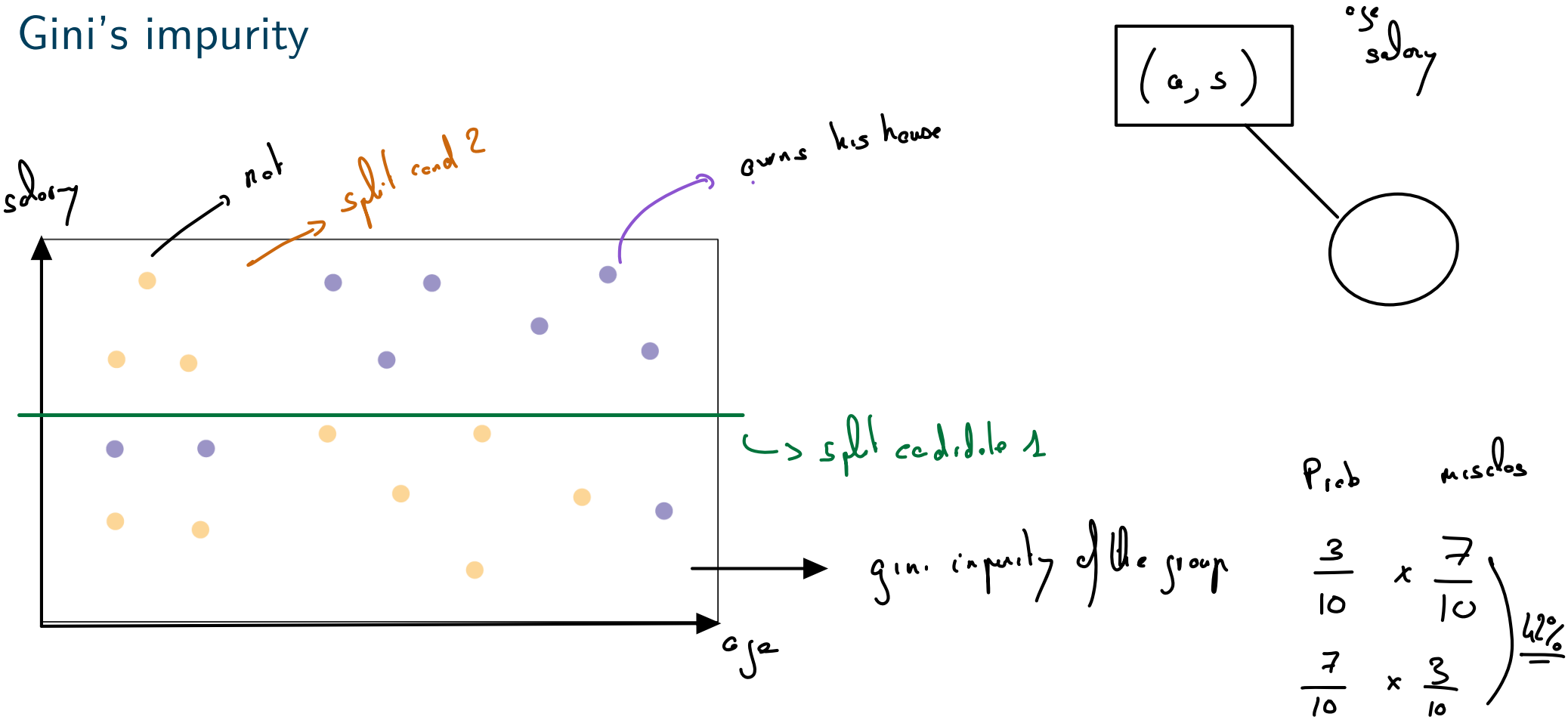




How to chose the best cut ?

- 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.

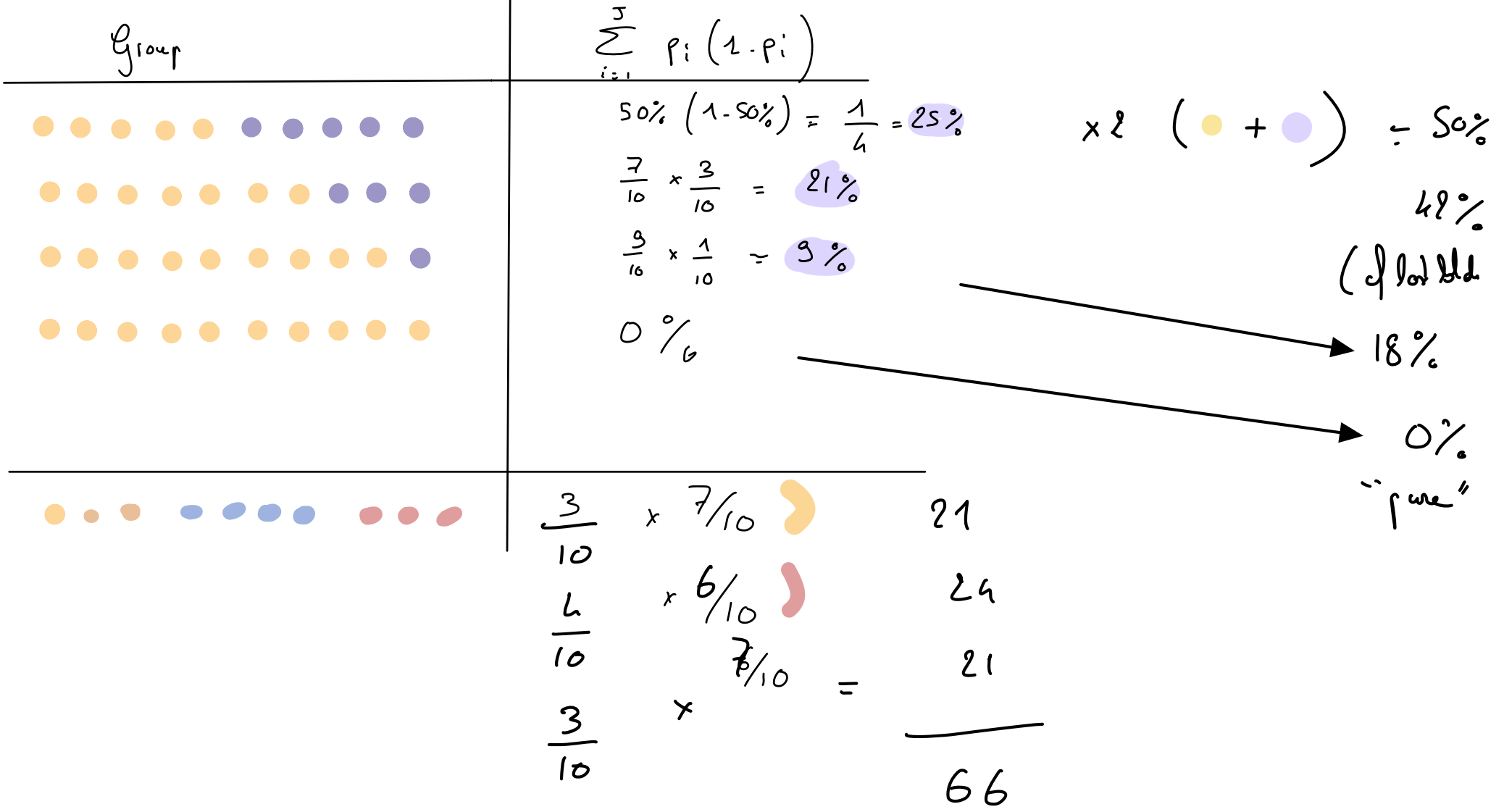
Gini's impurity



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**.

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

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



Idea : a good split is one that makes both parts homogeneous in terms of output values.

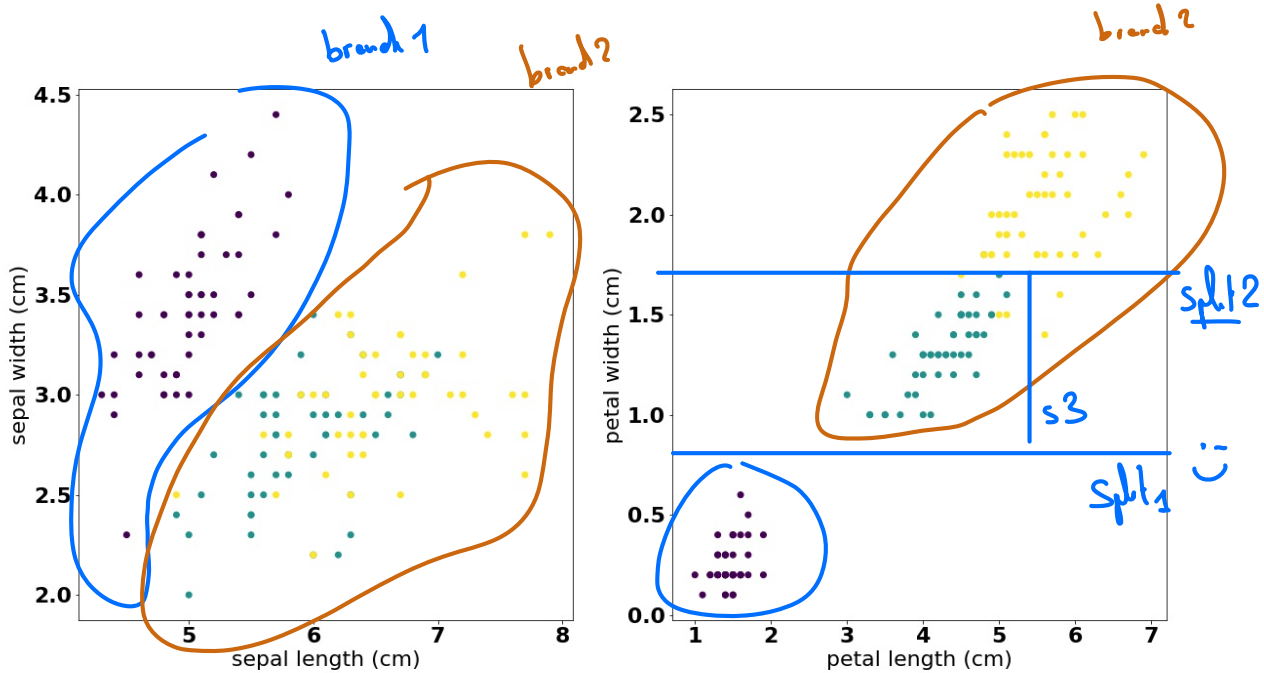
Example: Iris Dataset



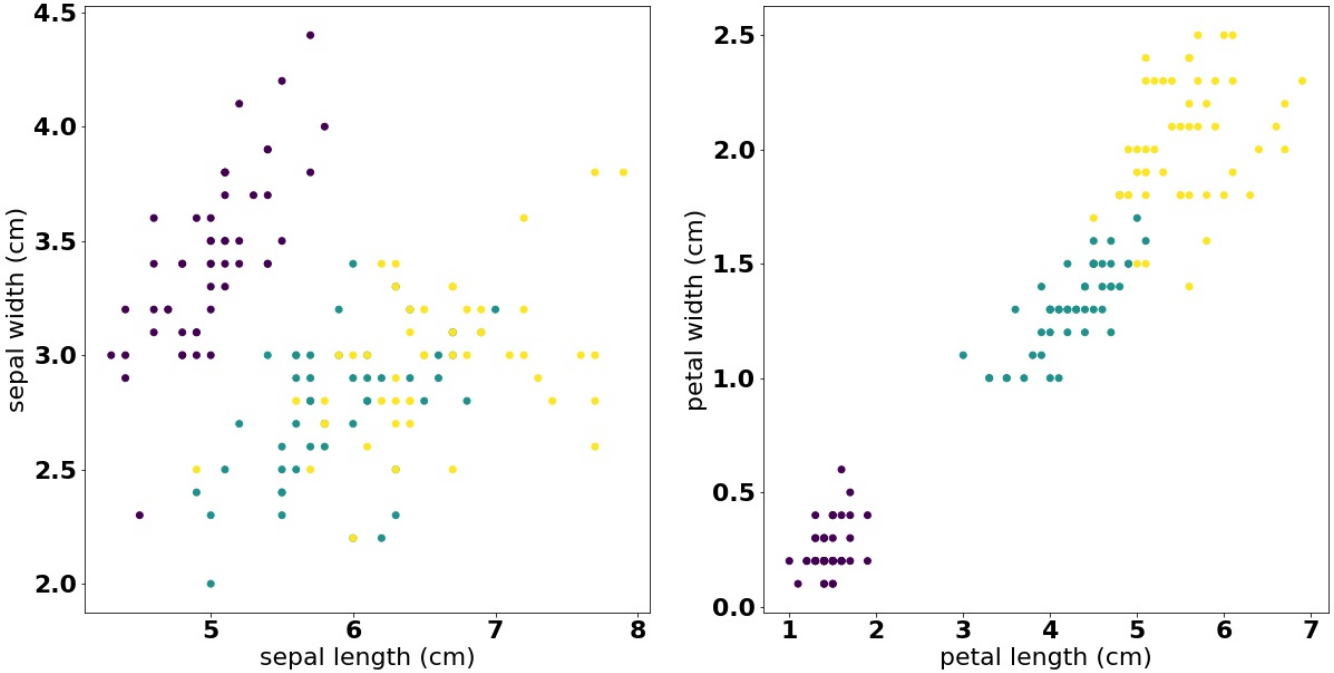
Figure: Iris: setosa, versiocolor, virginica

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']*



Exercise: Guess Classification tree for Iris Dataset



In pratice : Scikit Learn

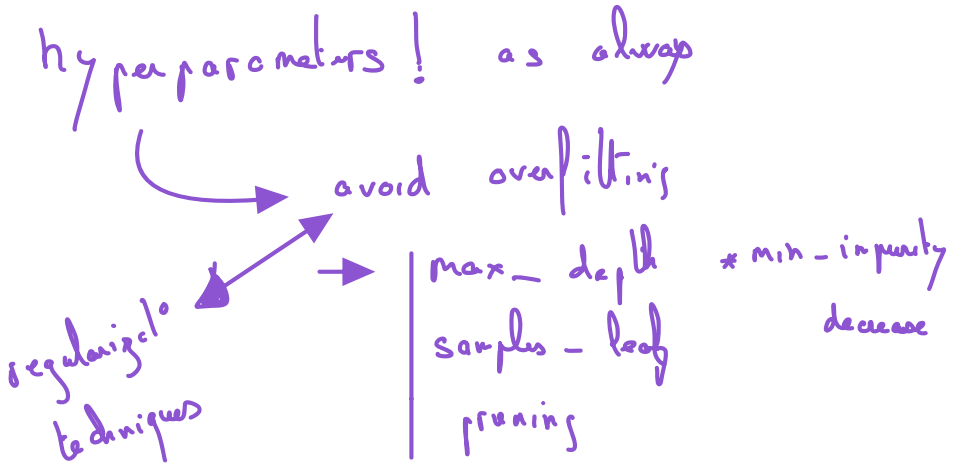
Universal Python library for Machine Learning:

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

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

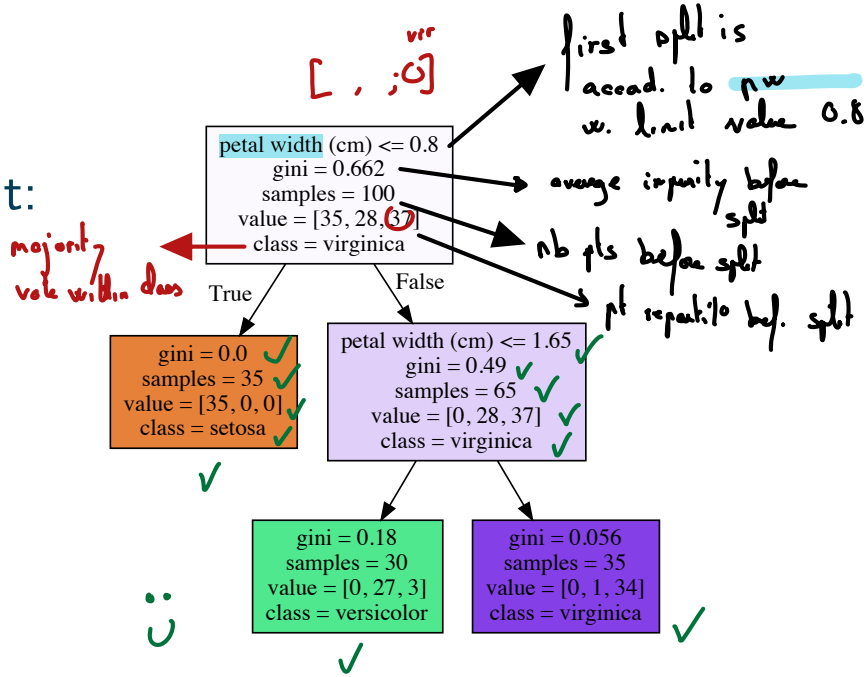
Example: Iris Dataset

What do we need to specify ?




```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, [redacted], 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

Woodop.

Decision trees and Supervised Learning

1. The depth is "learned" in DT ✗
2. The depth is a hyperparameter ✓
3. I use the validation set to find hyperparameters ✓ (cv)
4. There is no train set for Decision Trees ✗

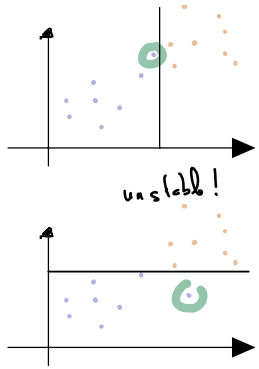
Which of the following statements are true about the construction of a decision tree?

1. The same feature cannot be used twice consecutively" ✗
2. The same feature cannot be used twice overall" ✗
3. I can use a pair of features if it gives me a better split ✗
4. I want to find the split that has minimal impurity ✓ obj for fit
5. To define a new split, I only use one example ✗

Which of the following statements are true about Decision Trees?

1. They are very stable ✗
2. They provide an interpretable approach ✓
3. They are able to approach the "optimal function" for nearly any data distribution (e.g. beyond linearly separable data) ✓
4. They work well for a high number of observations ✓
5. They do not work for Regression ✗ they do

large d → large risk :

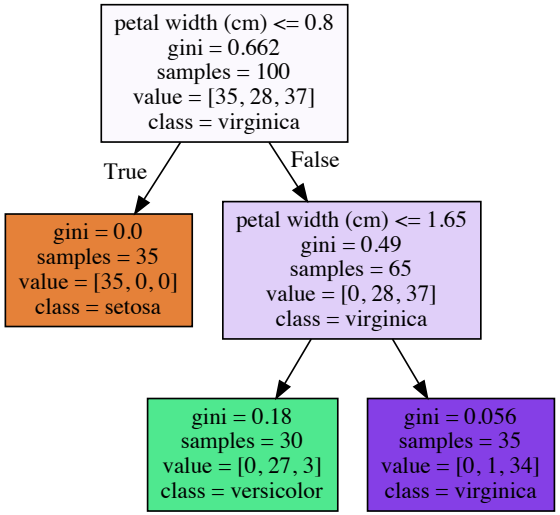


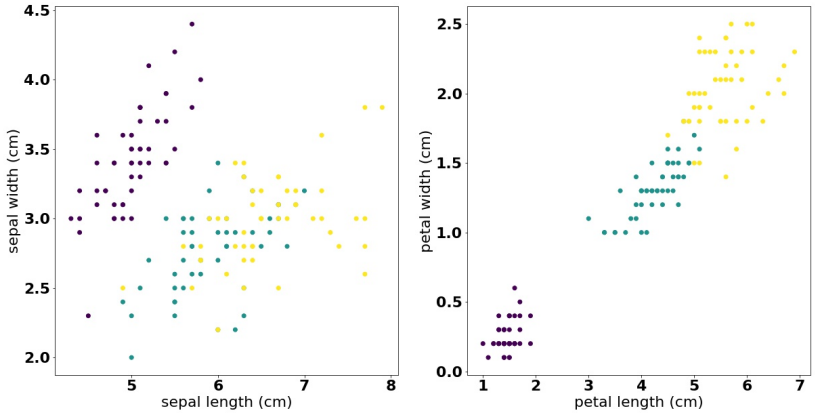
rich less → risk of overfitting

(≠ linear regression)

Example: Iris Dataset

Output:





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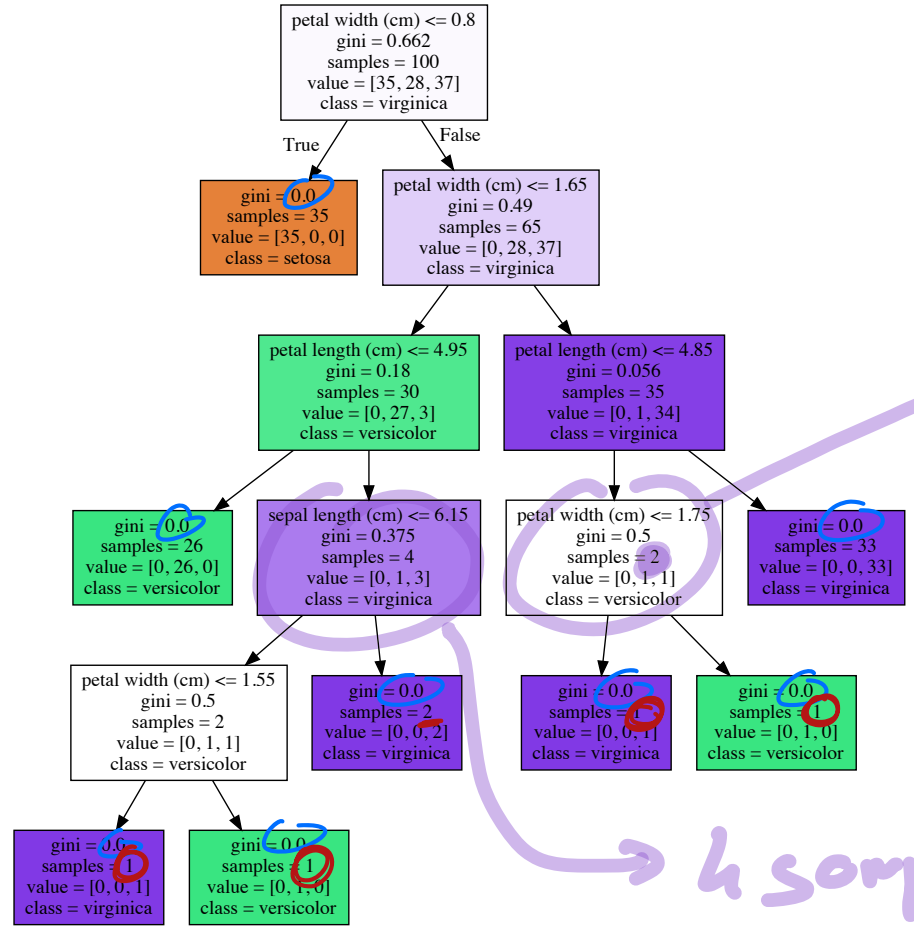
Returns:
(array([4.8, 3.1, 1.6, 0.2]), 'setosa')

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)
```



2 samples

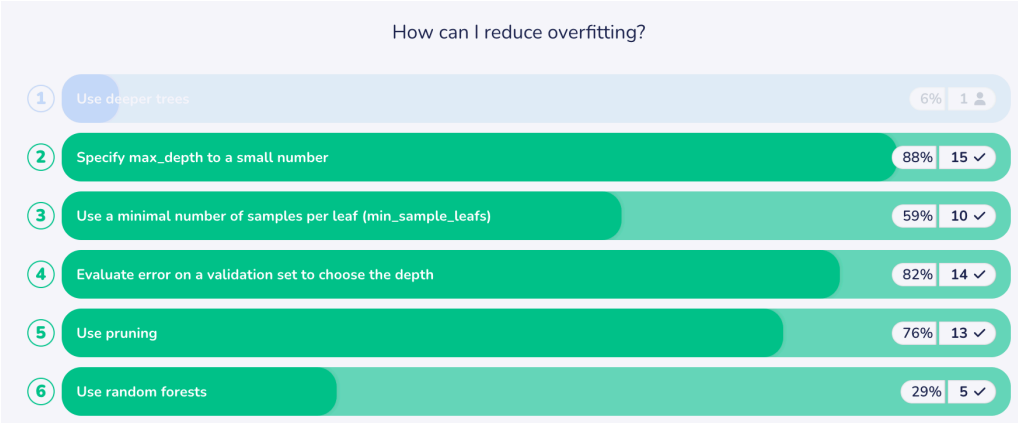
4 samples

5 nodes w 1 or 2 pts :-

- When does the algorithm stop then ? → gini = 0 on all nodes
- What do you think about it ? → overfitting risk

Stopping / Pruning

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

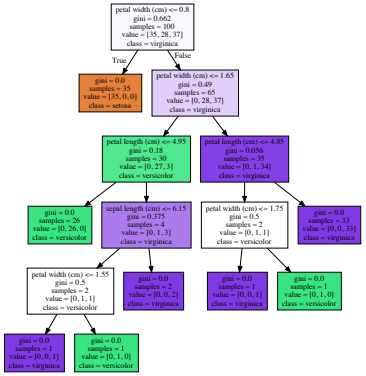


To avoid this problem, we can reduce the complexity of the trees:

1. Stopping rules
   - Set a minimum number of samples inside each leaf. ✓ e.g. 5
   - Set a maximum depth. ✓
2. Pruning
   - Reduced error pruning.
   - Cost complexity pruning. prune

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

Summary:

* how to predict w. a tree ✓
* how to fit a tree.
  → choose a criterion (Gini, Var) ...
  → iteratively find the best split

Pros:

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

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 ✓
4. Biased if some classes dominate ✓

* ⊕ → crossval
  pruning ; max depth, min_sample_ ; etc

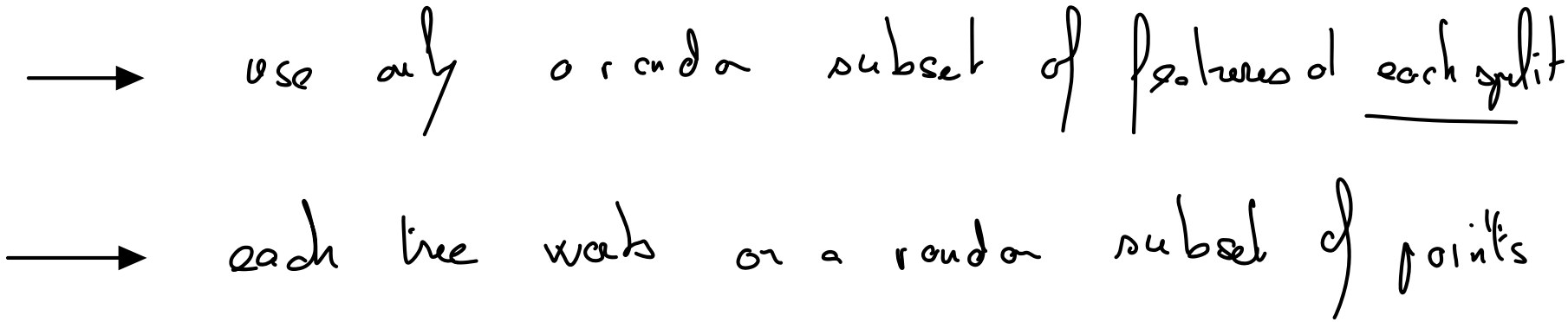
Solution : Using Random Forests !

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 ?



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 ?

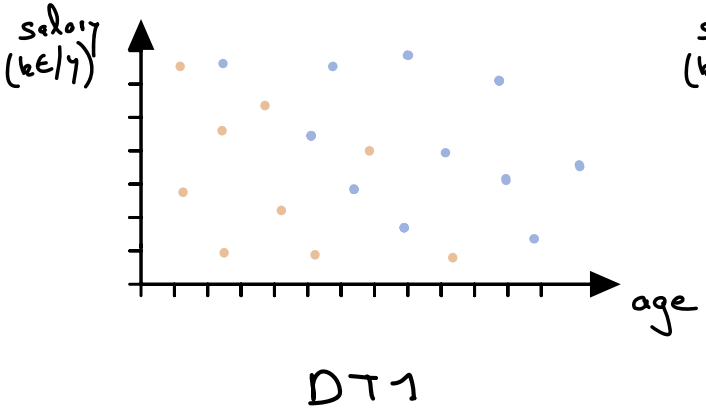
- Instead of the most important features, search the best feature among a random subset (ntry).
- Work on subsets of data (bootstrap=True).
- More `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestRegressor.html`

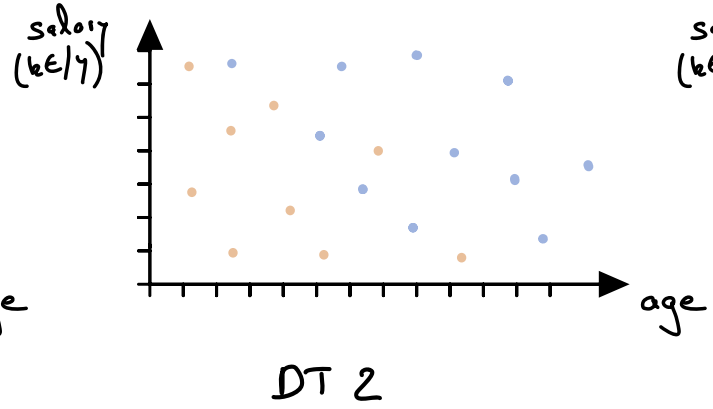
```
# Creating and fitting a Random Forest
from sklearn.ensemble import RandomForestClassifier

plt.figure(figsize=(20,10))
clf = RandomForestClassifier(n_estimators = 100,
                             max_depth=3, bootstrap = True,
                             random_state =43)

clf.fit(X_train,y_train)
```

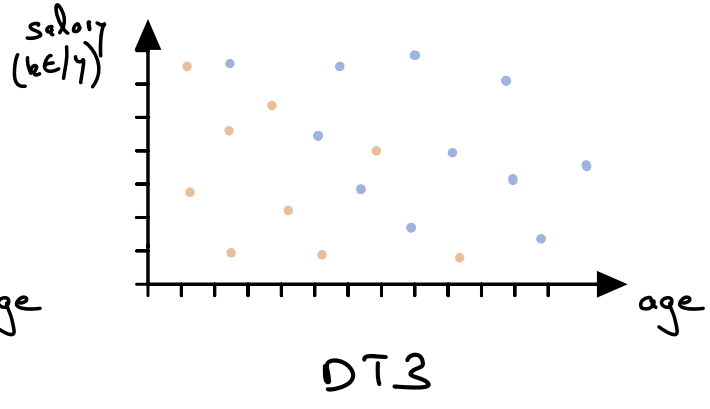
How to aggregate ? How to interpret a Random Forest ?

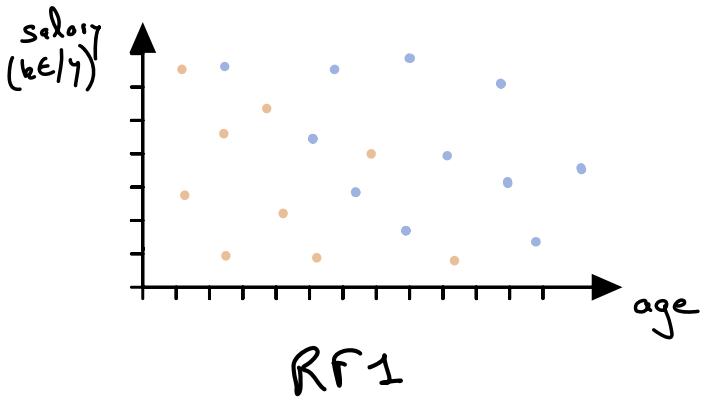
Aggregation

We using a voting or averaging process !



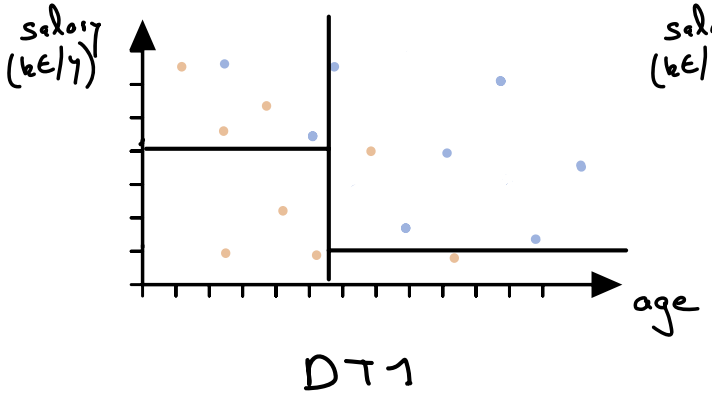


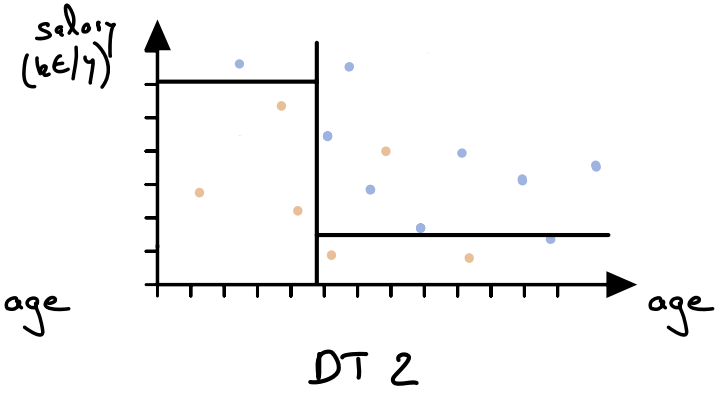


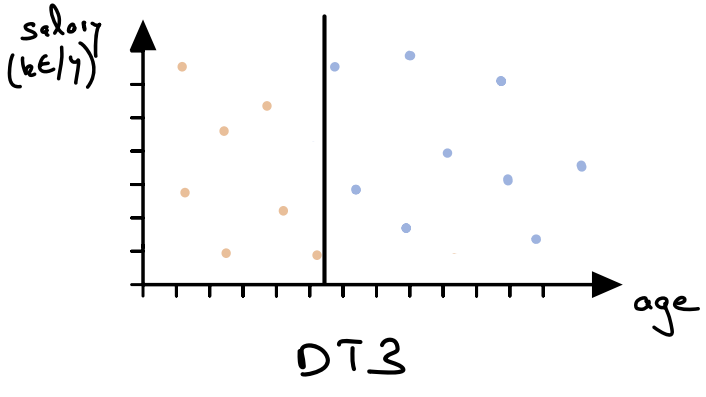


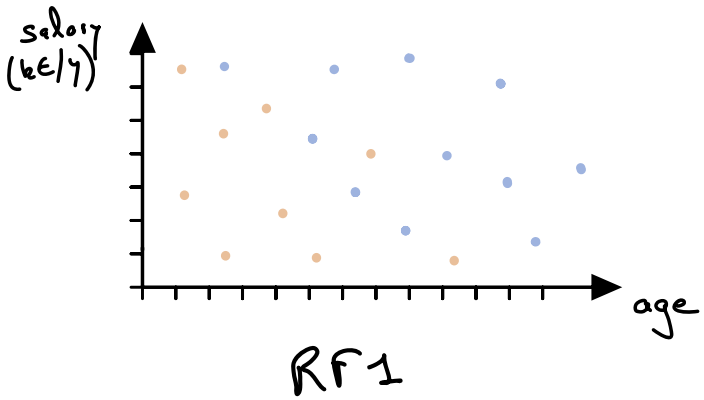
Aggregation

We using a voting or averaging process !



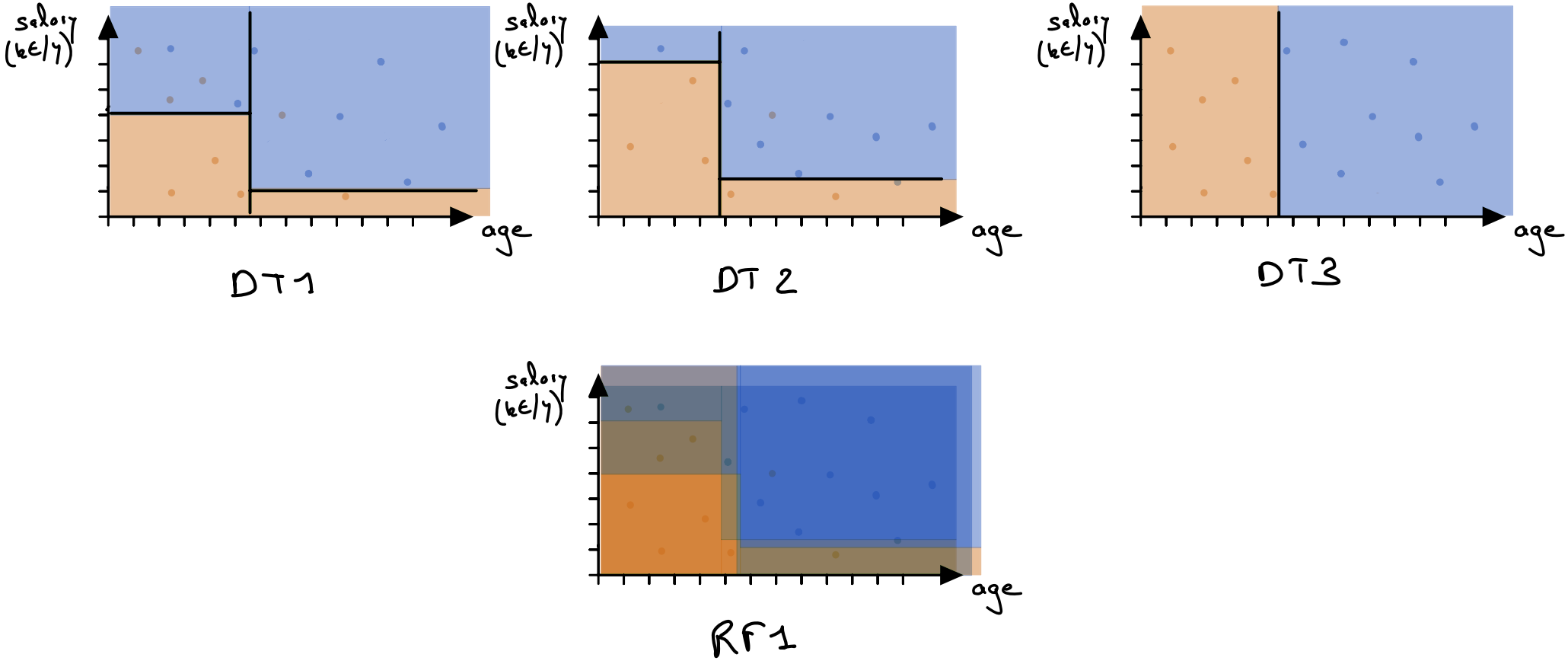






Aggregation

We using a voting or averaging process !



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.

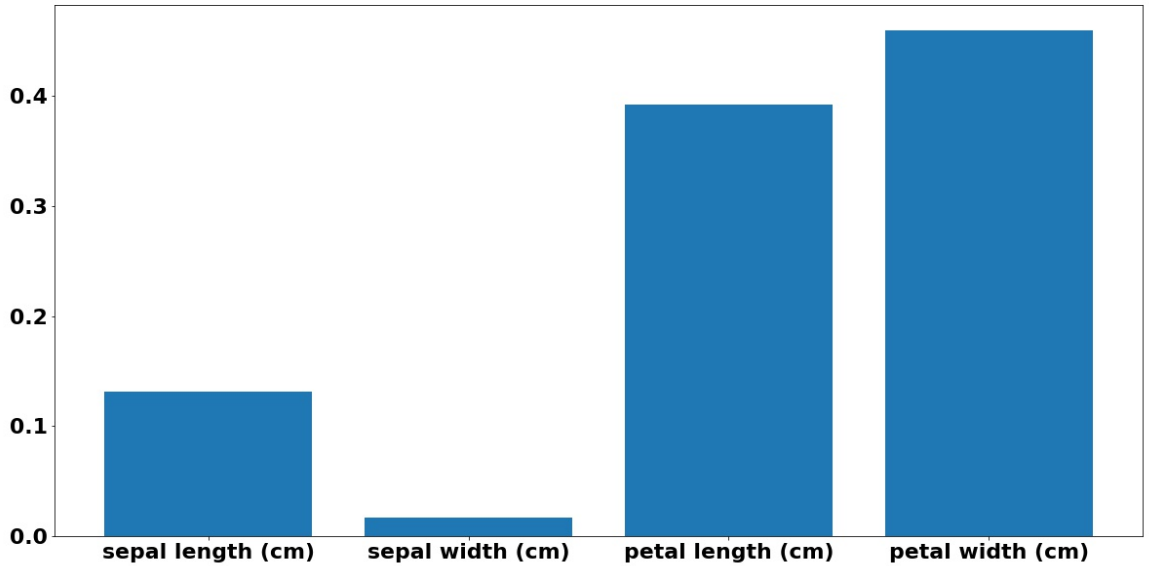


Figure: Feature importane output for a Random Forest Classifier in Python

Comparison with decision trees

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.
5. Bonus : supports multiple outputs!

RF Cons:

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

What about Regression ? works the same with Regression Trees

Questions?

Boosting

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`

Bonus: Multiple Outputs

- **Goal:** predict several outputs simultaneously
- **Solution:**
  - each leaf contains a value for each output
  - to chose the splits, we use a (weighted) average of the impurity of each output.

Bonus: complexity

Total complexity for one decision tree:

Worst case:

$$O(n^2 d)$$

Balanced case:

$$O(nd)$$

Tips

- Decision trees tend to overfit: limit the depth or use `min_samples_leaf` (5 is a good initial pick)
- Visualize the tree with a small depth first
- Balance your dataset: trees tend to be biased towards dominating class.

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.