ML, Decision Trees and Random Forests
Data science Certificate

Aymeric DIEULEVEUT

April 2025

1. Introduction to Supervised Learning

What you are not allowed to forget

For any algorithm $X \rightarrow \square \rightarrow Y$ how do I train / what training is

2. Decision Trees

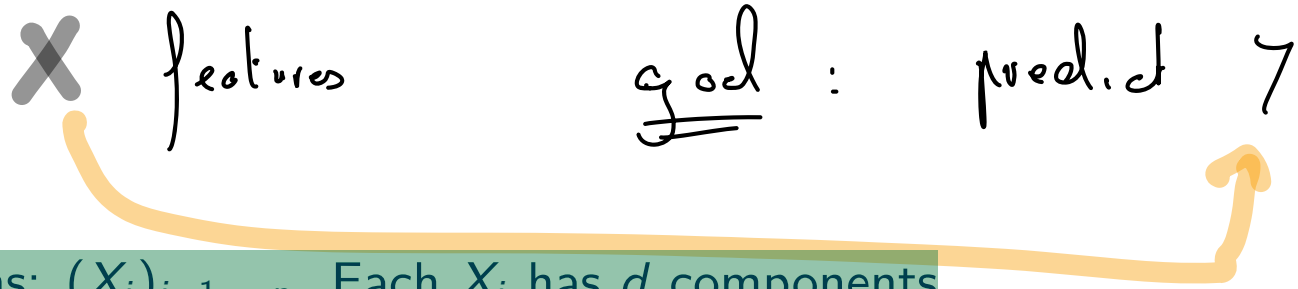
Dec Tree

3. Random Forests

Neural Networks

Outline

A Reminder on Supervised Learning



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

d = number of features

n = number of obs.

3 Examples:

- Iris Dataset:

  prediction iris type from 4 features

- MNIST:

  predicting a digit from its image/pixels

- House price prediction

  X = (sq footage; sq footage balcony; floor; neighborhood; days of sun)

  5 features

Example 1: House price Prediction - Regression

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

House price Prediction dataset

- 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.

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

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.

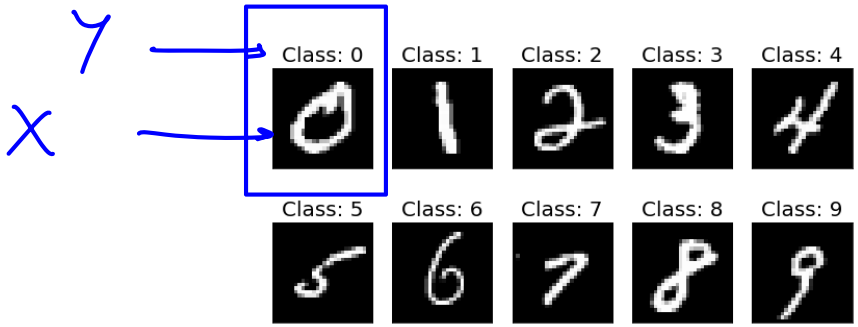
- 50 points per class

  $\rightarrow$ $n = 150$

- 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

60k

$$n = 60000$$

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

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

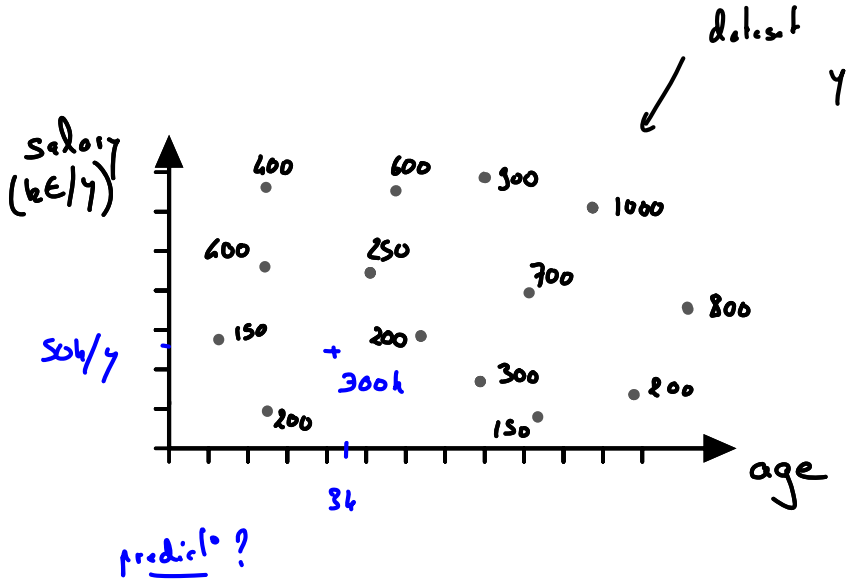
Summary of those three datasets

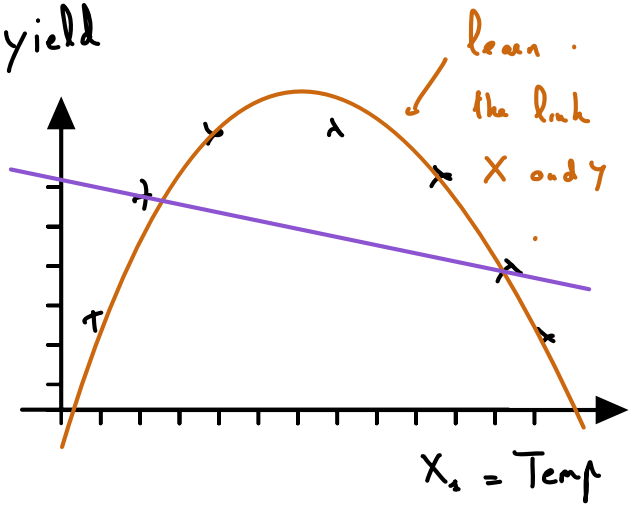
	Iris	MNIST	House price prediction
Number of examples n	150	60k	1560
Number of the features d	4	784	81
Type of the features	quanti	pixels → quantit	quantit / qualitative
Space $\mathcal{Y}$	3 classes	$\{0, \dots 9\}$	$\mathbb{R}$
Task	classifi	classificde	regress°

size dataset $\simeq 600$. $\simeq 60$ M $\simeq 100.000$

Toy datasets

- In regression:

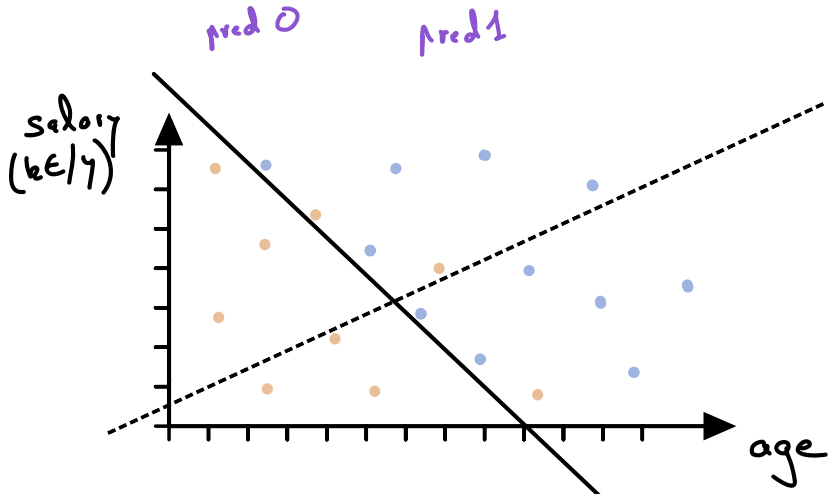




→ used a lot

d=1 : $y \in \mathbb{R}$

- In classification:



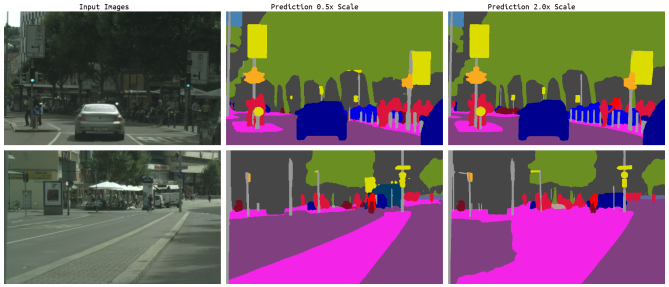
owns his house 1

rents his house 0

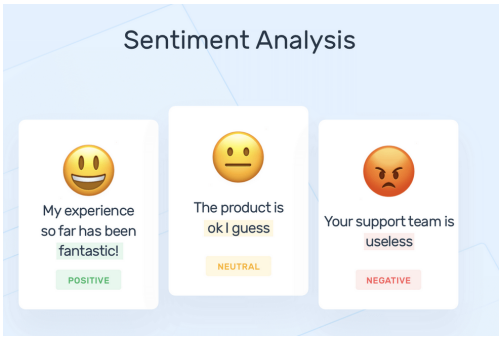
→ used a lot : d=2, $y \in \{0,1\}$

More examples

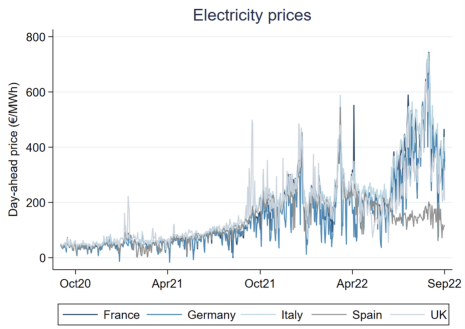
Spam detection



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 $(X, Y) \sim \mathbb{P}$.

Main ML assumption: Dataset (X_i, Y_i) i.i.d

indep. identically distributed.

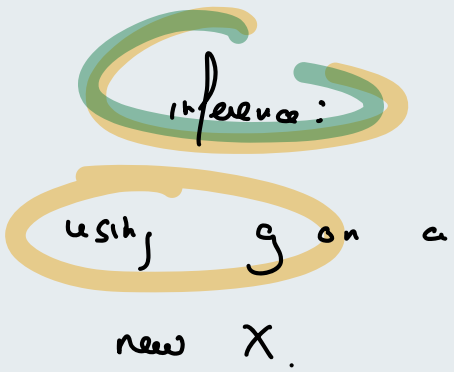
⚠ Be careful if distribution of the phenomena changes

Take aways compiled

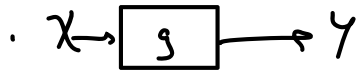
Supervised Learning

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 $(X, Y) \sim \mathbb{P}$.



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



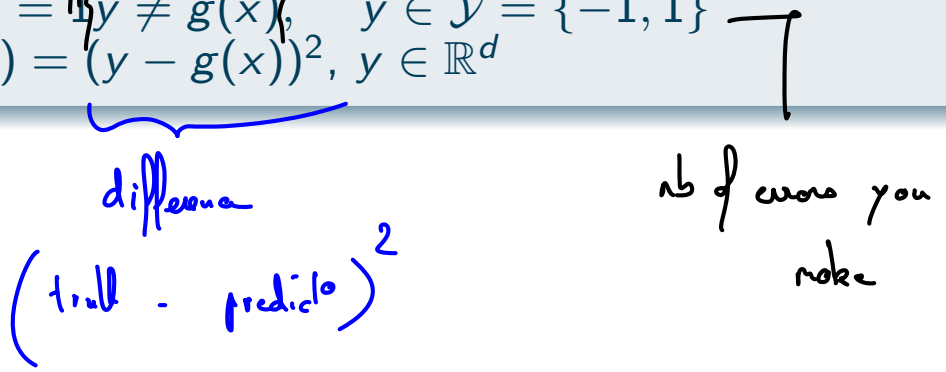
How to **quantify the quality** of a predictor?

$\rightarrow$ introduce a risk function.

Loss function, Generalization Risk and data-dependent predictors

Loss Function

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



Loss function, Generalization Risk and data-dependent predictors

Loss Function

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

Risk of a Decision Rule = average loss

g classifier / regressor.

- Risk: $R(g) = \mathbb{E}[\ell(Y, g(x))] = \int \ell(y, g(x)) d\mathbb{P}(x, y)$, e.g.: $(X, Y) \sim \mathbb{P}$
  - 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.

Find g that has a small Generalization risk.

Goal in ML: predict well on new data points — unseen in the dataset ⟶ this is what the generalization risk measures.

Loss function, Generalization Risk and data-dependent predictors

Loss Function

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

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.

⚠ 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.

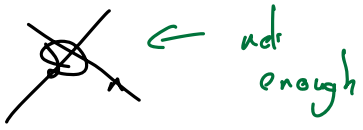
Some high level messages:

* what SML is !
* a few examples
* inductive thinking is — what learning is

Key assumpt° in ML modelling — data is iid, follows a fixed distrib

Approach: use a dataset $\mathcal{D}_n$ to learn a predictor $\hat{g}$.

overfitting } → we want $\hat{g}$ to be good on a new point.



Supervised Learning: Summary

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): $g : \mathcal{X} \to \mathcal{Y}$
- Loss: $\ell(Y, g(x))$
- Risk: $R(g) = \mathbb{E}[\ell(Y, g(x))]$

Numerous methods:

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

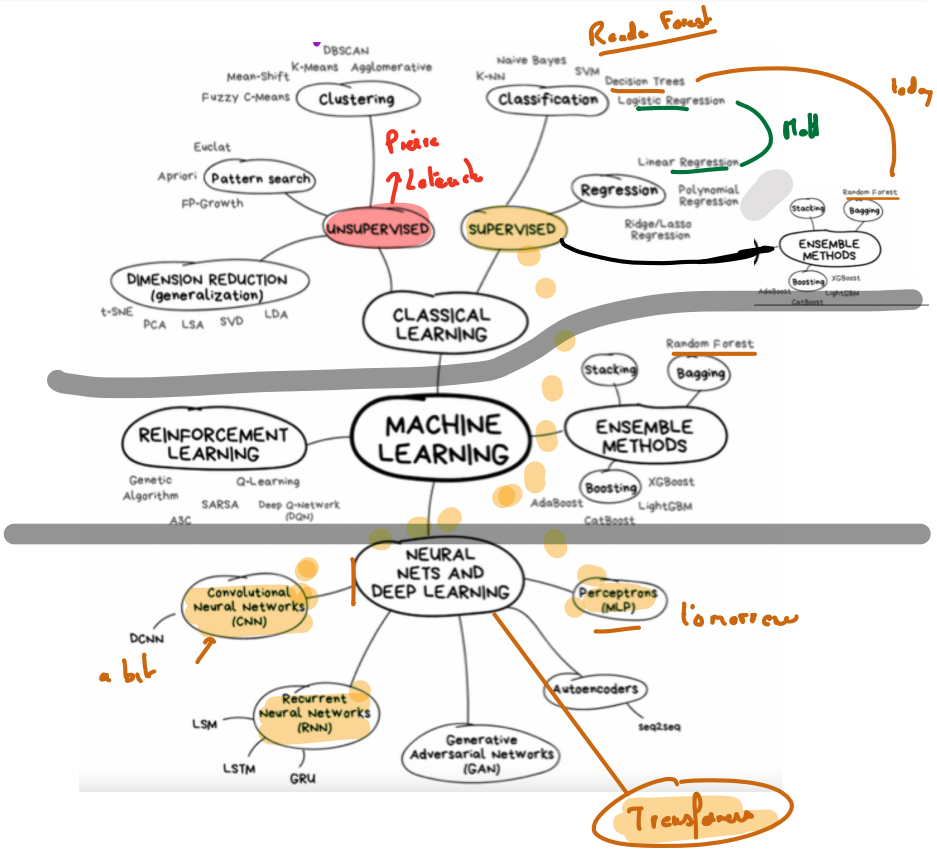


Figure:

Roadmap towards Understanding machine learning!

1. Understand conceptually how to train a model.

→ how to learn "weights"

→ what fitting is

→ overfitting – generalize

solo

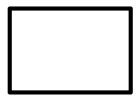
validation

or cross validation

valid for any □

---

2. Opening some □



Linear Reg → DT → RF → NN

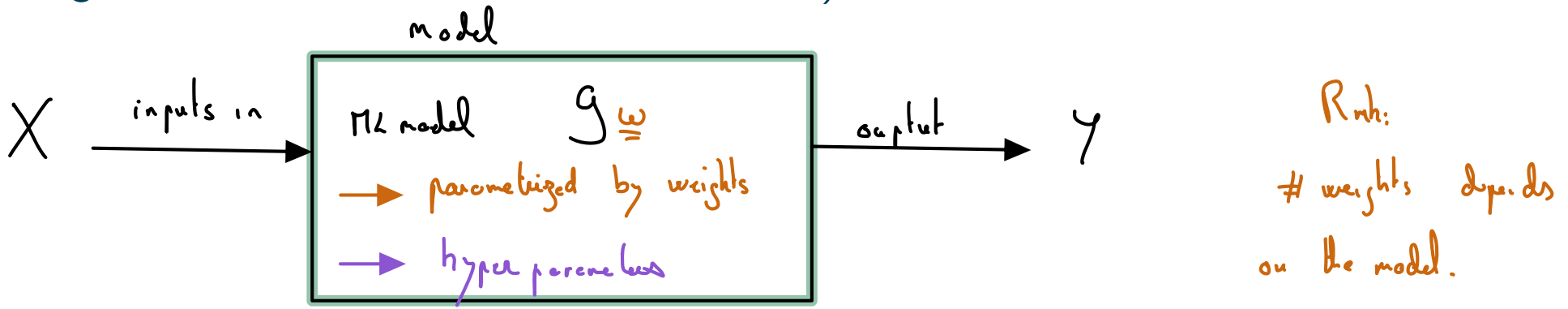
useful to pick

S / A / I

Training Pipeline

1. Fitting

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



Linear regression on House price prediction

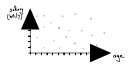
$$g(X_{surf}, X_{bdc\,surf}, X_{pcon}, \dots) = b_0 + \omega_1 X_{surf} + \omega_2 X_{bdc} + \dots$$

weights to be learned.

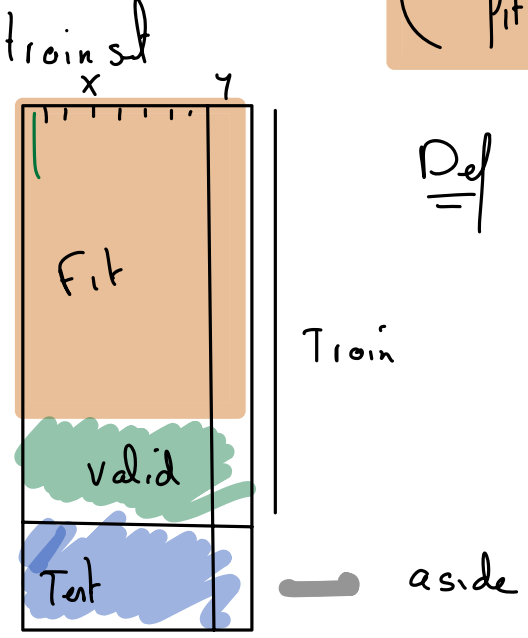
→ # : 81

Fitting is done on a part of the training dataset

find a function that behaves well on it



(X_{fit}, Y_{fit})



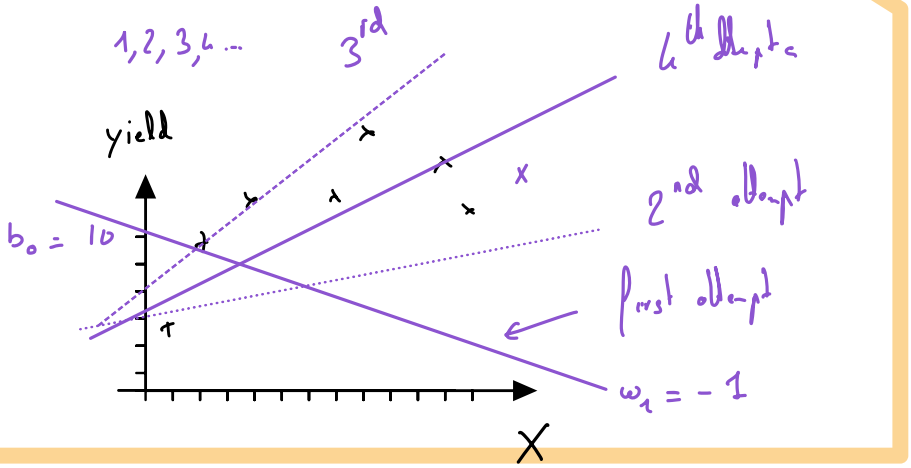
Def: **Fitting** = finding ω such that g_ω is good on (X_{fit}, Y_{fit})

→ typically minimize the empirical risk

$$\omega \mapsto R(g_\omega) = \frac{1}{n_{fit}} \sum_{i=1}^{n_{fit}} \ell\left(g_\omega(X_{fit,i}), Y_{fit,i}\right)$$

quality of prediction (w.r.t. ℓ) on point i of fit set

How to fit? main algorithm is "incremental improvement"



Fit: → 95% time: "incremental improvements"

e.g. NN;
linear regression*;
logistic regression; SVM; etc

→ 5% time: specific algorithm.

→ DT!, RF!

(* or closed form formula $(X^TX)^{-1}X^TY$)

Fitting a method

Demo url (Lab): https://colab.research.google.com/github/adieulev/Certificate-DS-2025/blob/main/Labs/MWE_ML_init_student_version.ipynb

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

# Setting aside 10% of the data
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.9, 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))
```

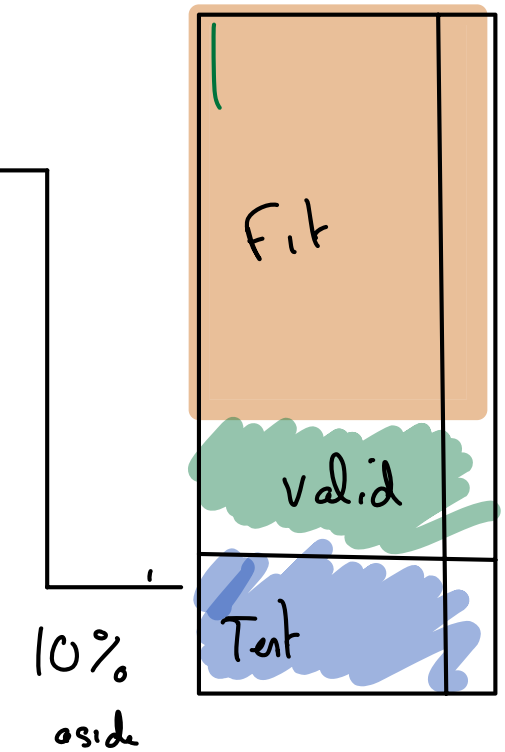


Figure: Importing a dataset

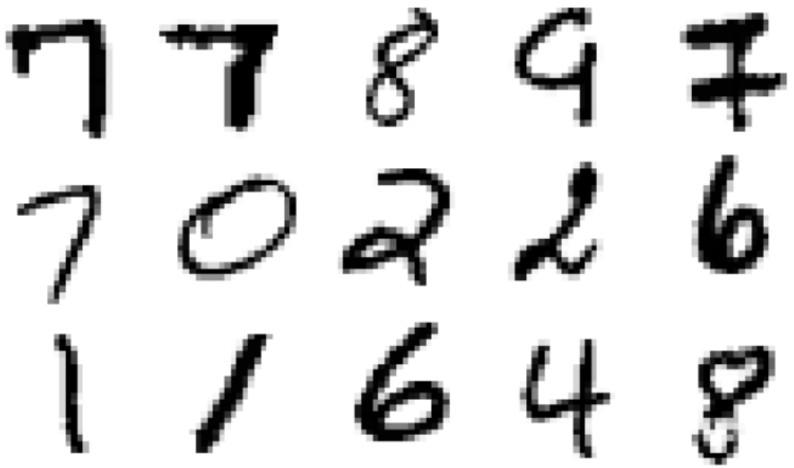


Figure: Digits

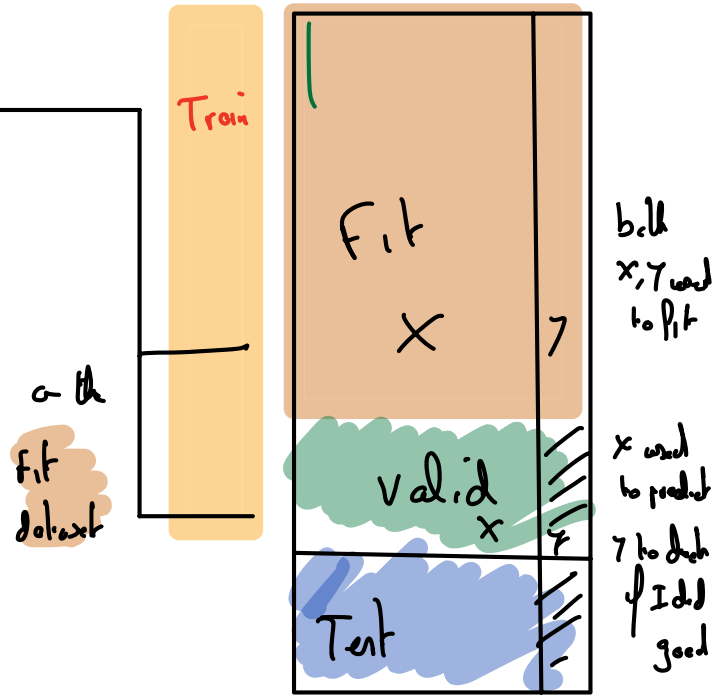
Fitting 3 methods

```
X_fit, X_val, y_fit, y_val = train_test_split(X_train,  y_train,
                                              test_size=0.2, random_state=42)

from sklearn.tree import DecisionTreeClassifier

dt_clf = DecisionTreeClassifier()
dt_clf.fit(X_fit, y_fit)
```

define an instance of a decision tree

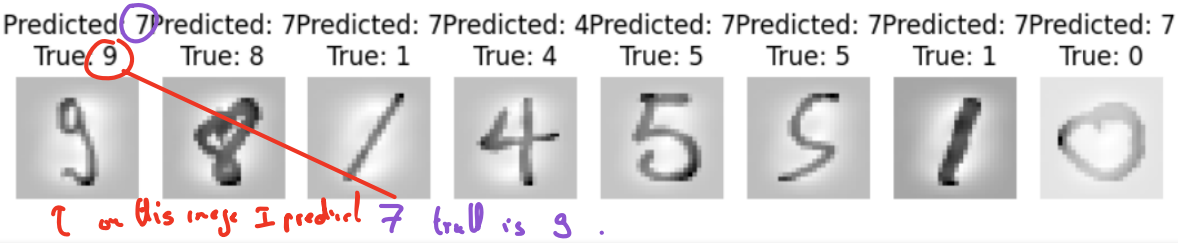
used what 80% of ML for 2010 - 2015

our DT is fitted : it has learned on the fit dataset




```
DecisionTreeClassifier()
```

```
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')
```



I on this image I predicted 7 truth is 9.

0s
```
from sklearn.ensemble import RandomForestClassifier
```
0s
```
rf_clf = RandomForestClassifier(n_estimators=10,random_state=42)
rf_clf.fit(X_fit, y_fit)
```

define my object

Fit!

all happens in "fit" !

```
RandomForestClassifier(n_estimators=10, random_state=42)
```

HYPER PARAMETERS

You need to chose them

```
from sklearn.linear_model import LogisticRegression

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

Fit!

```
LogisticRegression(multi_class='multinomial', random_state=42)
```

Looking at the accuracy

Obtain Accuracies on dataset to fit (train accuracy)

```
[25] print(
         f"On the dataset used to fit, the decision tree has "
         f"{100 * dt_clf.score(X_fit, y_fit):.1f}% accuracy"
     )
     print(
         f"On the dataset used to fit, the random forest has "
         f"{100 * rf_clf.score(X_fit, y_fit):.1f}% accuracy"
     )
     print(
         f"On the dataset used to fit, the logistic regresssion has "
         f"{100 * log_reg.score(X_fit, y_fit):.2f}% accuracy"
     )
```

↑ my DT ↑ get its accuracy → specific dataset

```
On the dataset used to fit, the decision tree has 100.0% accuracy
On the dataset used to fit, the random forest has 99.8% accuracy
On the dataset used to fit, the logistic regresssion has 100.00% accuracy
```

Train accuracy (fit accuracy) — not reliable metric of your generalization risk!!

Obtain Validation Accuracies

```
[26] print(
         f"On the dataset left aside for the fitting part, the decision tree has "
         f"{100 * dt_clf.score(X_val, y_val):.1f}% accuracy"
     )
     print(
         f"On the dataset left aside for the fitting part, the random forest has "
         f"{100 * rf_clf.score(X_val, y_val):.1f}% accuracy"
     )
     print(
         f"On the dataset left aside for the fitting part, the logistic regresssion has "
         f"{100 * log_reg.score(X_val, y_val):.2f}% accuracy"
     )
```

look on the validation dataset!

```
On the dataset left aside for the fitting part, the decision tree has 77.6% accuracy
On the dataset left aside for the fitting part, the random forest has 88.8% accuracy
On the dataset left aside for the fitting part, the logistic regresssion has 87.57% accuracy
```

DT is worse than RF or Logistic Reg

→ ♡♡♡. To estimate the generalization risk; I use

Wooclap time!

a few points (validation set) that the model has not seen during fit.

1 Allez sur wooclap.com

2 Entrez le code d'événement dans le bandeau supérieur

Code d'événement
TAMXAU

1 Envoyez @TAMXAU au 06 44 60 96 62

2 Vous pouvez participer

Désactiver les réponses par SMS

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 (fit) set for that ✓ — yes typically often necessary, not sufficient
6. The goal is to predict well on the train (fit) points — not only
7. The balance interpretability/speed/performance depends on the method ✓ ↔ and applied
8. I assume my training data (fit + validation + test) to be representative (iid) of a phenomenon with distribution P ✓✓ !

What is the role of fitting, e.g., in

```
rf_clf = RandomForestClassifier(n_estimators=10,random_state=4...
```

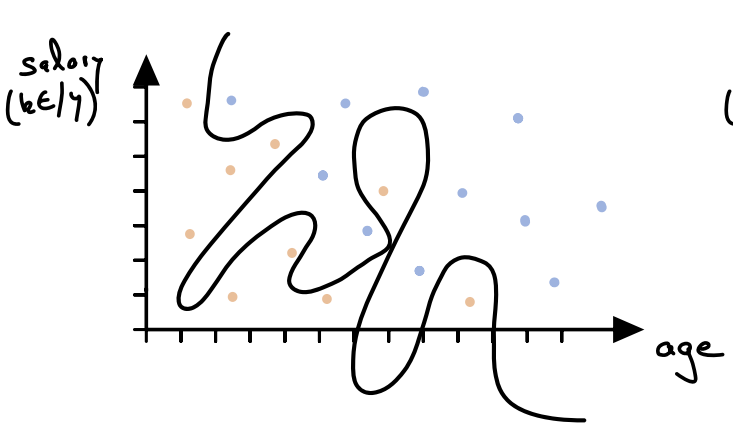
rf_clf.fit(X_fit, y_fit)

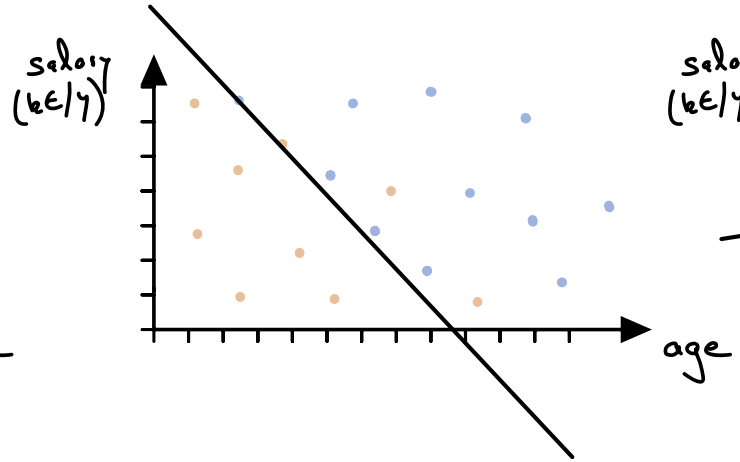
1. Finding the best parameters of the Forest/Treess ✓ — fit(w)
2. Finding the best hyperparameters (n_estimators) — fit — nope — use cross val for that
3. Predicting on a test point — nope — rf_clf.predict(X_test) to predict

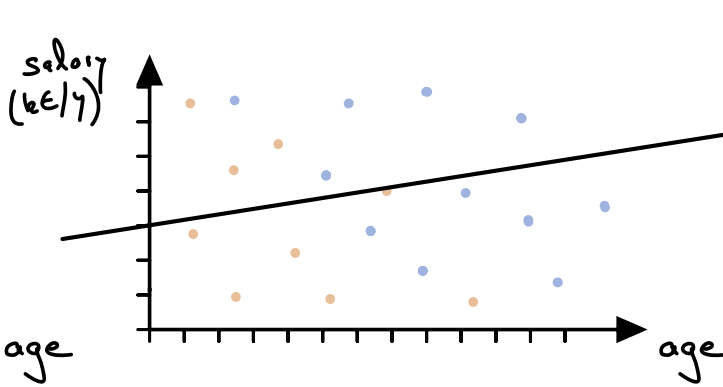
Caveat: Overfitting - Toy datasets

⚠ 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!!



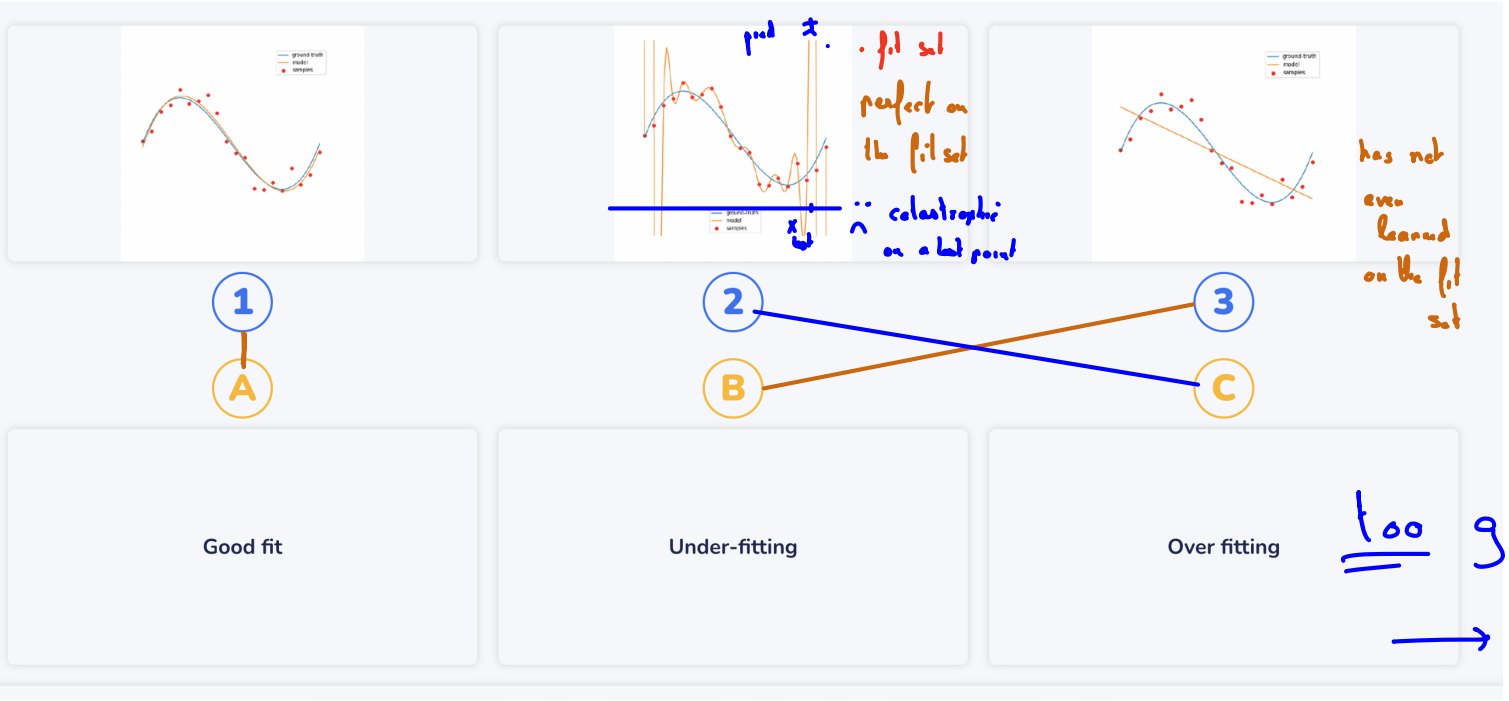




Fit error: 0 (perfect) | 15% = 3/20 pts | 50% 10/20 pts

Test error: higher (overfitting) | low (good fit) | very high (underfit)

💡 Need to focus on validation/test performance



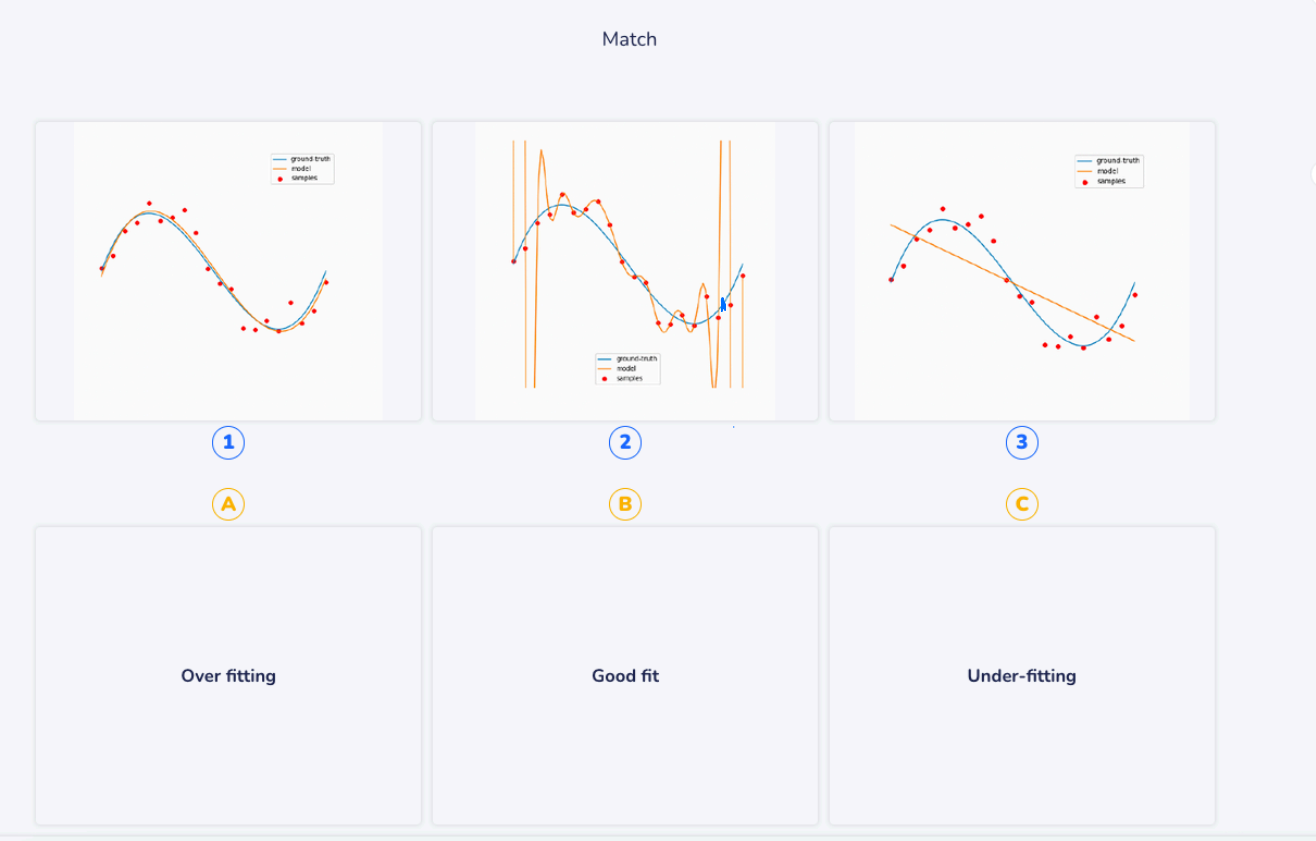
too good on the fit set

→ hallucinating on the test

Caveat: Overfitting - Toy datasets

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

💡 Ou

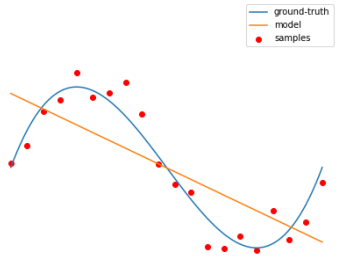


💡 Need to focus on validation/test performance

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

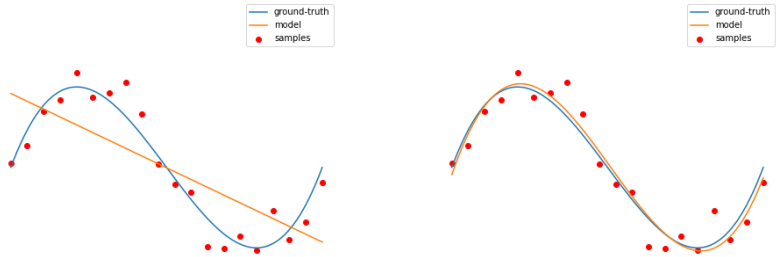
$\mathcal{C} =$
$\hat{R}_n(\theta_n^*)$
$R(\theta_n^*)$
Problem
Dim. of Θ

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



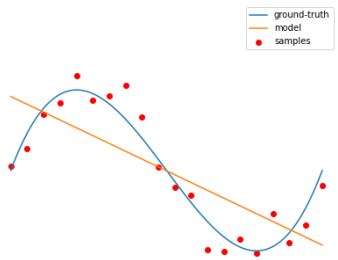
$\mathcal{C} =$	Affine functions
$\hat{R}_n(\theta_n^*)$	high
$R(\theta_n^*)$	high
Problem	Underfitting
Dim. of Θ	2

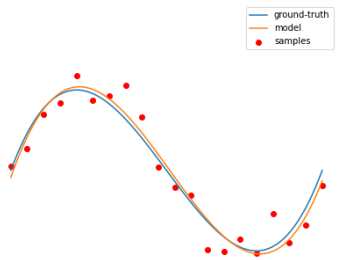
Underfitting and Overfitting depending on the choice of $\mathcal{C}$

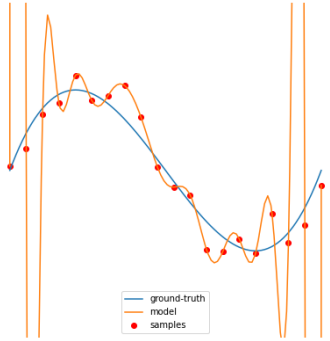


$\mathcal{C} =$	Affine functions	$\mathbb{R}_3[X]$
$\hat{R}_n(\theta_n^*)$	high	low
$R(\theta_n^*)$	high	low
Problem	Underfitting	All good
Dim. of Θ	2	4

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

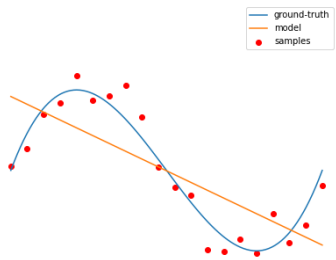


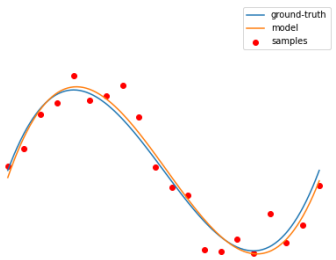


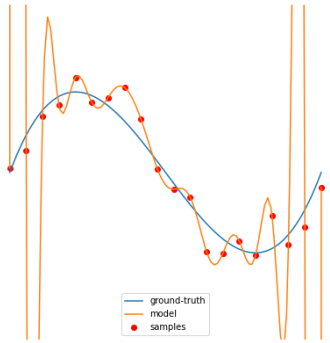


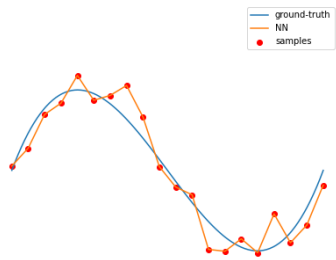
$\mathcal{C} =$	Affine functions	$\mathbb{R}_3[X]$	$\mathbb{R}_{19}[X]$
$\hat{R}_n(\theta_n^*)$	high	low	zero
$R(\theta_n^*)$	high	low	high
Problem	Underfitting	All good	Overfitting
Dim. of Θ	2	4	20

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

1. Training phase
2. Test phase
3. Deployment

1 model. how good is it

Training set (X_{train}, Y_{train})

TRAIN

FIT

VALID

TEST

Test

1 Fitting Phase

Goal : learn the parameters of the model on the (X_{fit}, Y_{fit})

2 Validation phase

Possible models & Hyperparameters

Goal: find an accurate predictor of the generalization error by estimation on validation data

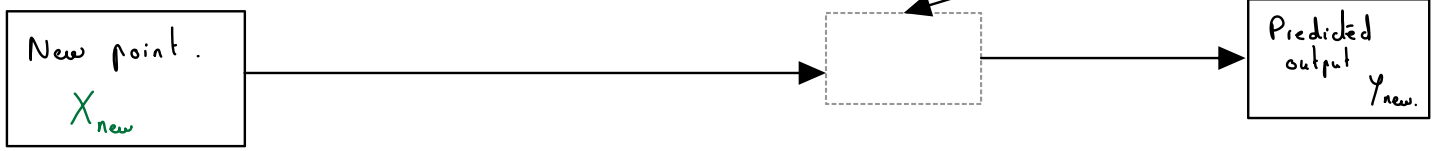
Choose the best model

Fitting algo.

Learns function $\hat{f}_n =$ [ ]

i.e. weight $\hat{w}$, bias $\hat{b}$

+ Cross validation → estimation of the generalisation

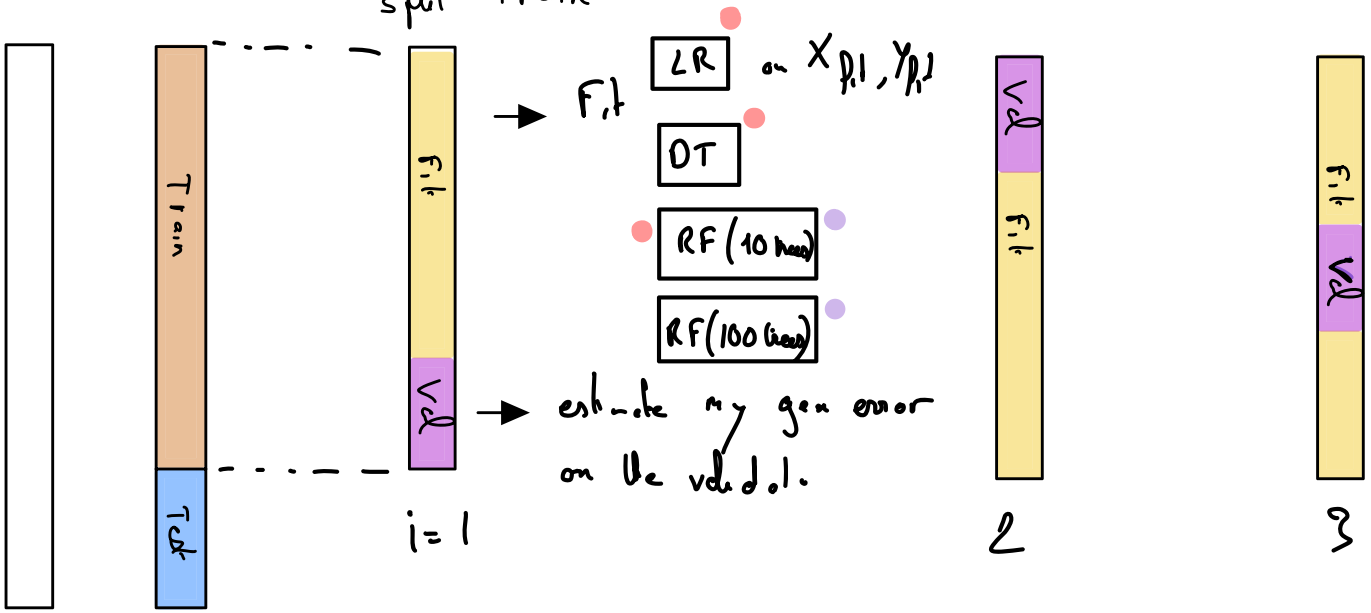


deploy the best model.

Cross Validation

Goal: select the best model / best hyperparam.

for i = 1 ... n_splits ← nb of splits,



I obtain for each model / hyperparam 1 estimate of the gen. error

→ average the n_split estimates

→ now you select a model / hyperparam

more reliable champion

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

av:

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]:

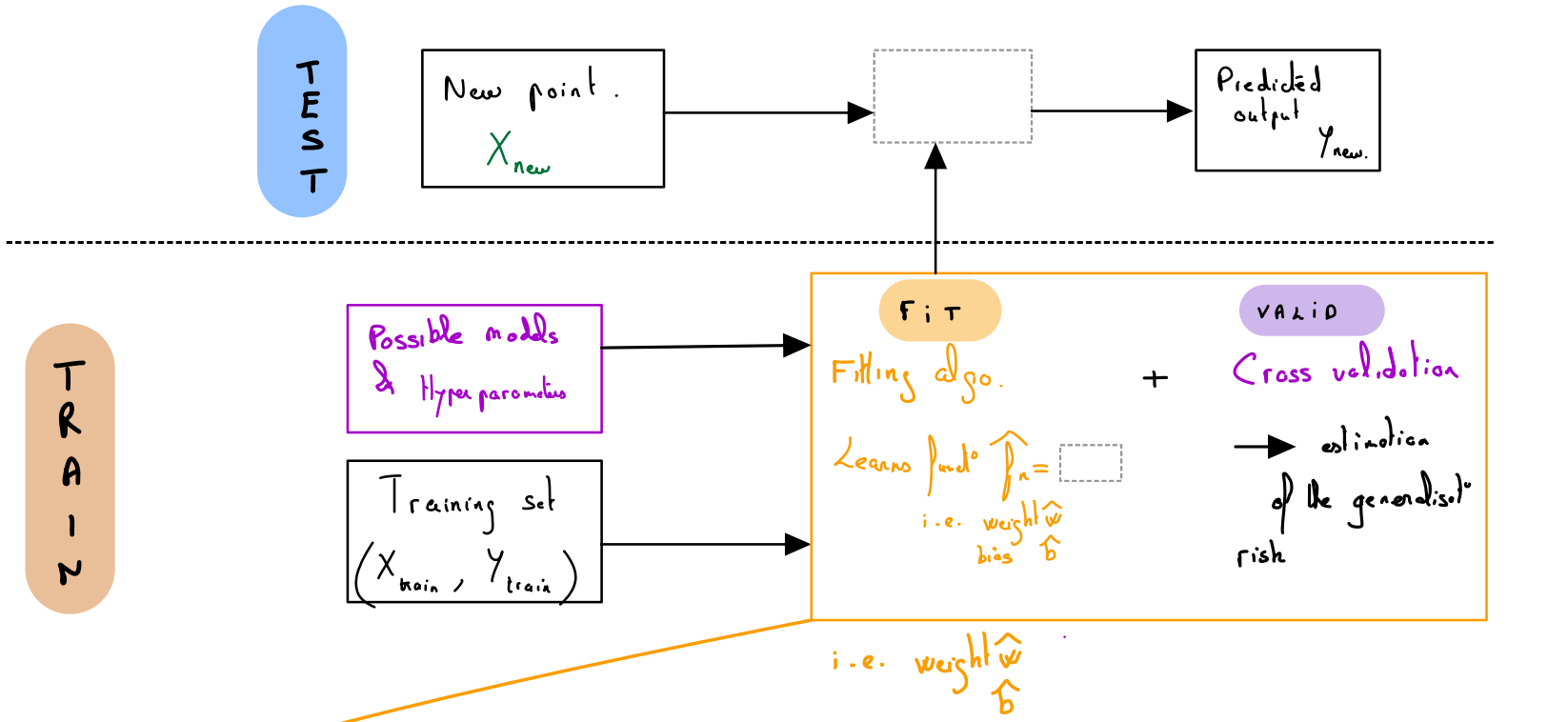
```python
pd.DataFrame(grid_search.cv_results_)
```

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



Learning: by GD.

Define a risk: ERM

$R\left(\hat{f}_n, X_{train}, y_{train}\right)$ - minimize it

Iteratively improve $\hat{f}_n$ within the class of allowed fct°.

take a training point X^p

compute $\hat{f}_n(X^p) = \hat{y}^p$

$X^p \rightarrow \hat{y}^p$

compare to y^p

improve the weights

$\times 10^6$.

SML -Summary

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

SML -Summary

1. Key concepts
   - Tasks
   - Methods
   - Overfitting and cr
2. Black box solution:

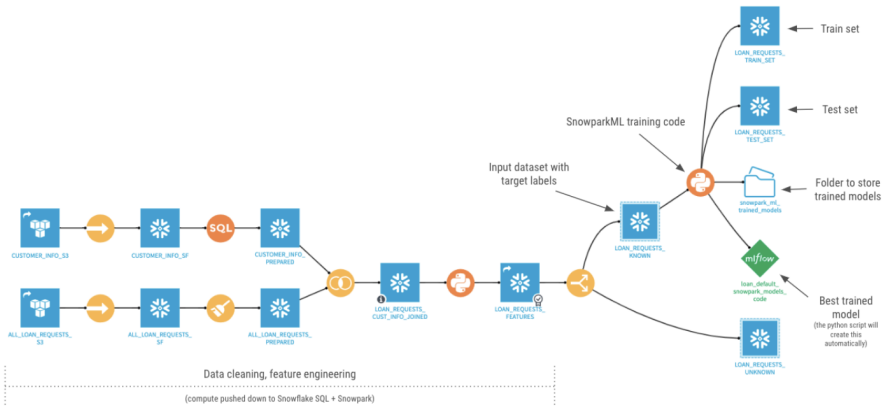


Figure: Dataiku

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

SML -Summary

1. Key concepts
   - Tasks
   - Methods
   - Overfitting and cr
2. Black box solution:

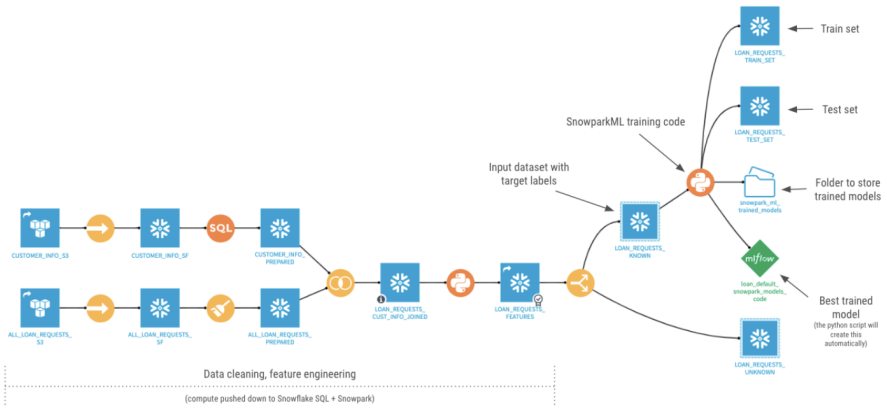


Figure: Dataiku

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

3. 💡 Our goal for today and tomorrow: **Opening the black box**
   → Understanding methods enables to better anticipate the best choice, limits, potential, etc.
   → Which method is suitable depending on Performance/Speed/Interpretability trade-offs
   → Better choices for hyper-parameters to be chosen

Wooclap time!

1 Allez sur wooclap.com

2 Entrez le code d'événement dans le bandeau supérieur

Code d'événement
TAMXAU

1 Envoyez @TAMXAU au 06 44 60 96 62

2 Vous pouvez participer

Désactiver les réponses par SMS

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 ✓ instability

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 → .fit
3. Find the best hyperparameters in terms of validation error ✓
4. Fit the model
5. Find the best parameters in terms of validation error → ? ✗

at the end of CV, you get a fitted model for the best model + hyperpa that is the best. in terms of valid.te error

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
```

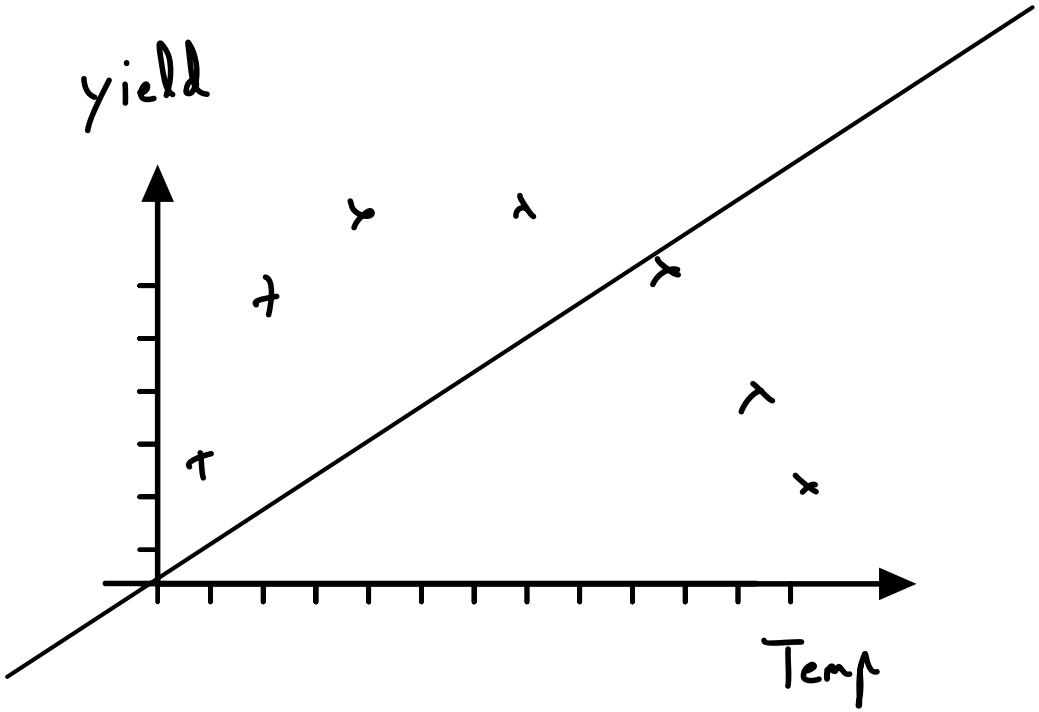
Out[18]:

	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

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
5. It computes 5 scores for each method, splittin the train data
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
9. 25 fits were performed overall
10. 5 fits were performed overall

Limits of Linear and logistic regression - towards DT



Linear regression : is bad here.

* the relationship between X (Temp) and Y is non linear
* if I have House price dataset with 81 features, I get a model w. 81 coefficients

DT

learn non linear relationships !

strong interpretability

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**

.fit
.predict

NN. $\rightarrow$ { .fit = incremental updates (Stoch gradient descent)
.predict $\longrightarrow$ what we have to understand tomorrow

Inference Phase

being able to predict from the free.

$X = (\text{age}, \text{precd}, \text{medical doctor})$

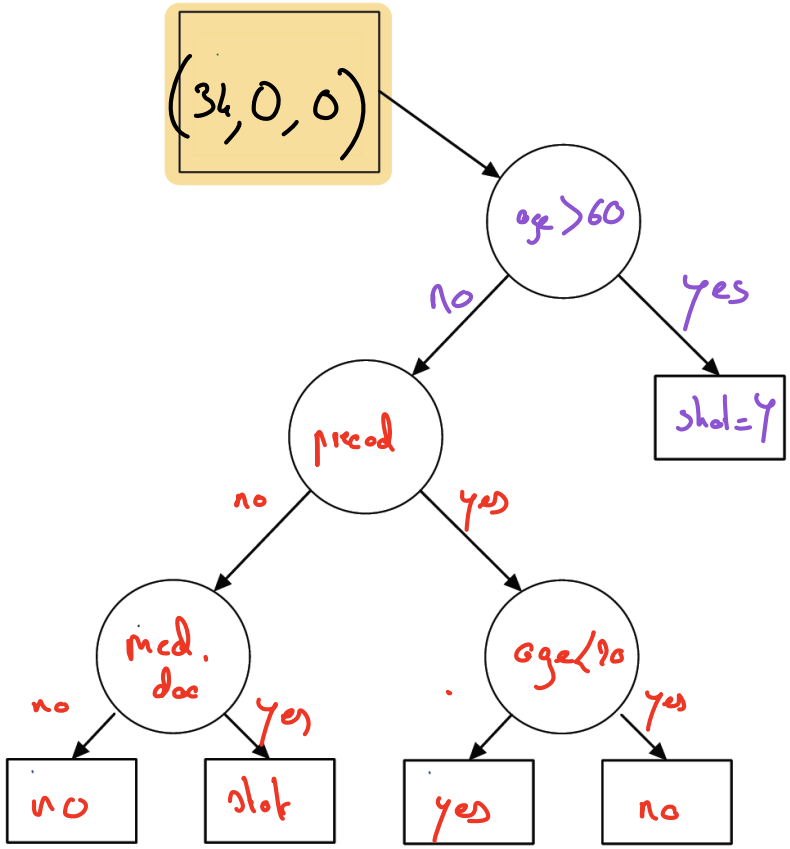
$\mathbb{R} \quad \{0,1\} \quad \{0,1\}$

$Y = \{$ get covid shot or not $\}$

- Root = observation = input

(16, yes, no)

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



What do we have to learn ⟶ list of questions

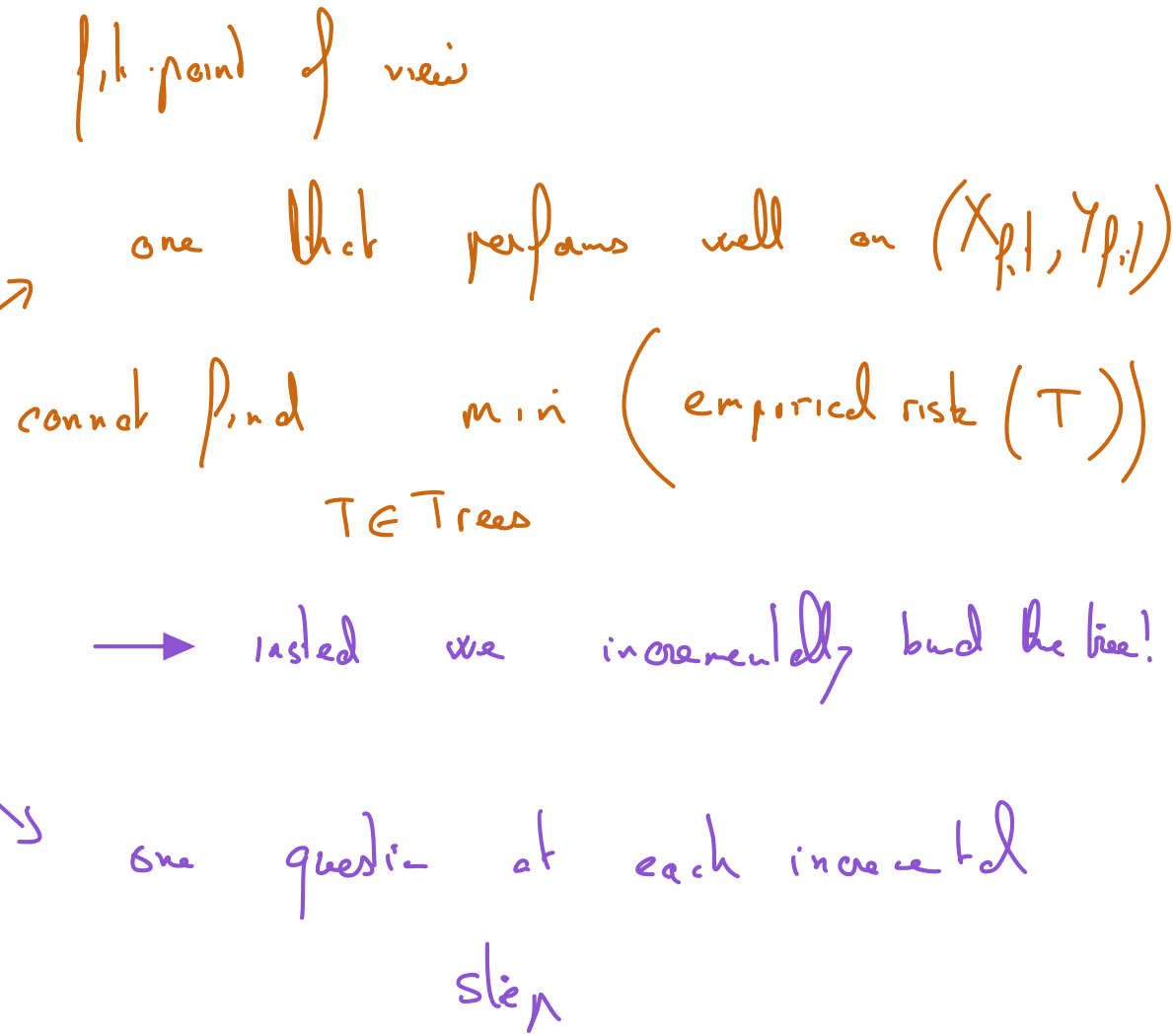
each question = {feature, threshold}

Training: how to build a tree.

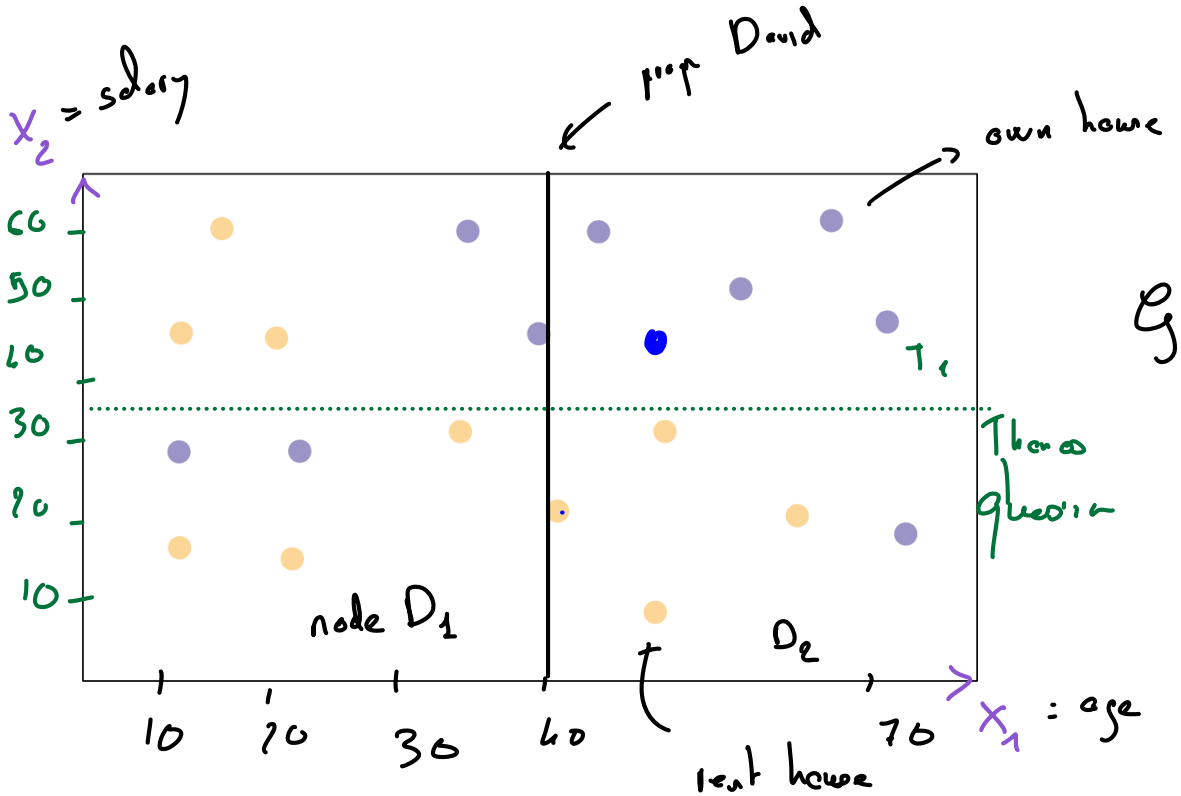
Key question !

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

What do you think?



Building trees : CART



	David's ?	Theo ?
D_1	6 ● 4 ●	T_1 3 ● 7 ●
D_2	4 ● 6 ●	T_2 8 ● 2 ●
Gini → D_1	0.4 × 0.6 = 24 %	0.3 × 0.7 ≃ 21 %
→ D_2	0.4 × 0.6 = 24 %	0.8 × 0.2 = 16 %
	48 %	37 %

key : criterion of quality ↑

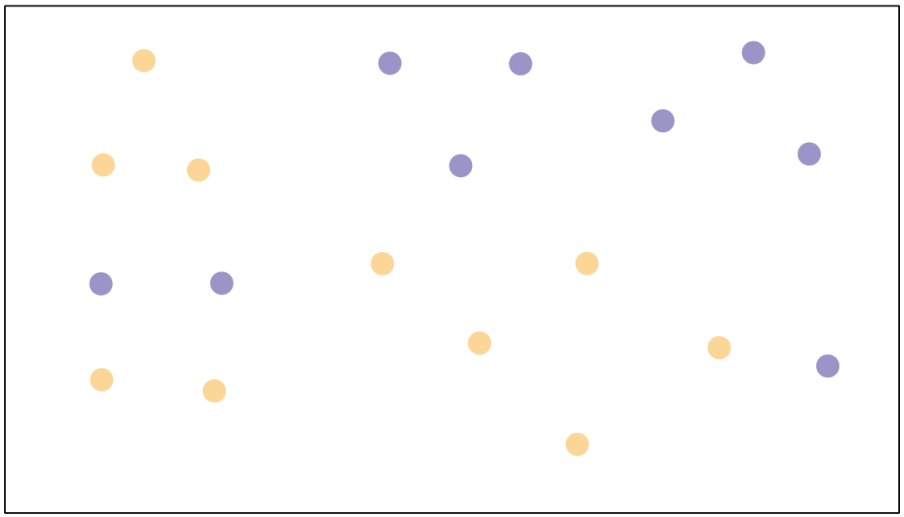
homogeneity within the splits

Gini's impurity : within each node ; $p_i(1-p_i)$

↑ p_i = probability of color ● or ●

select minimal impurity

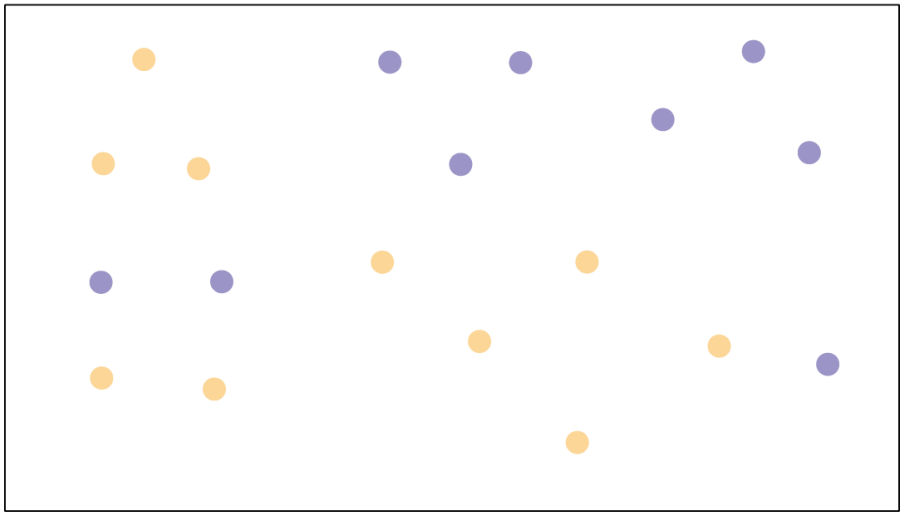
Building trees : CART



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**.

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

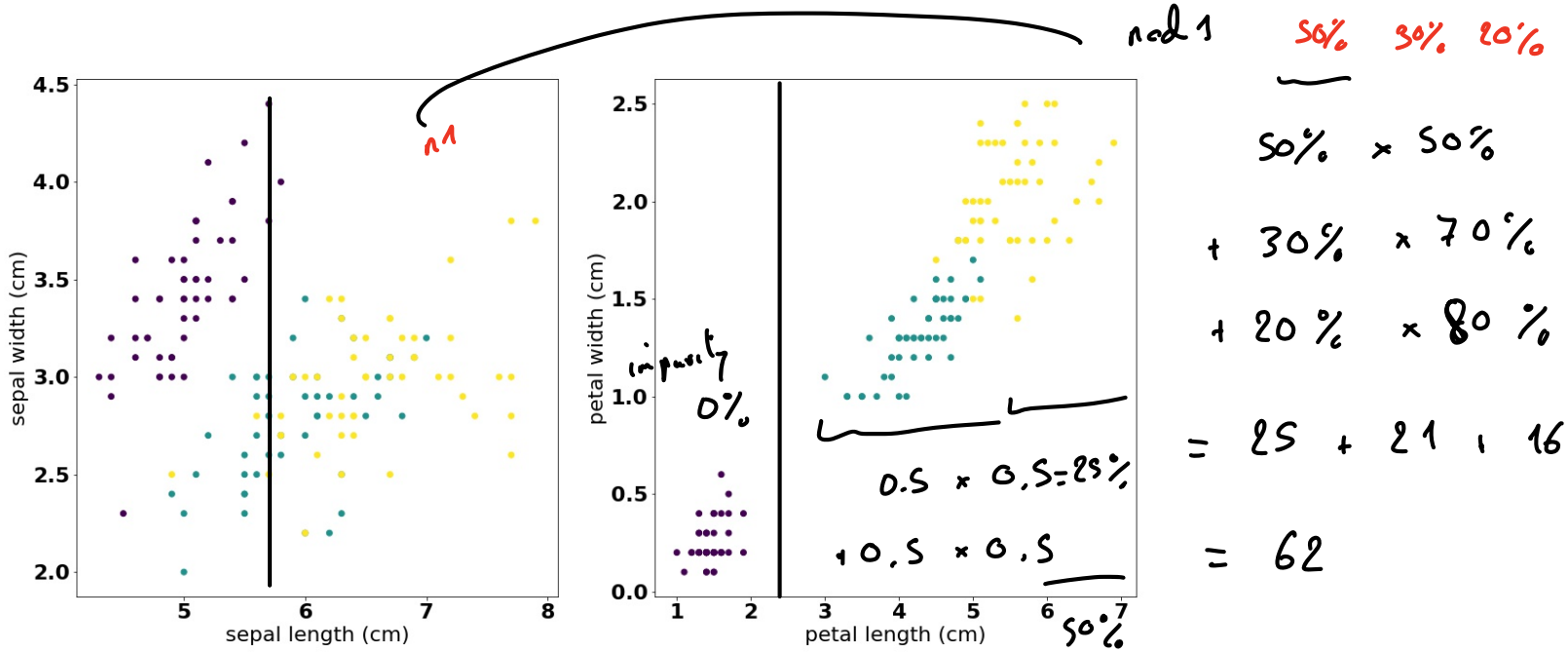
For two classes, related to the variance if classified as Bernoulli r.v..

Example: Iris Dataset

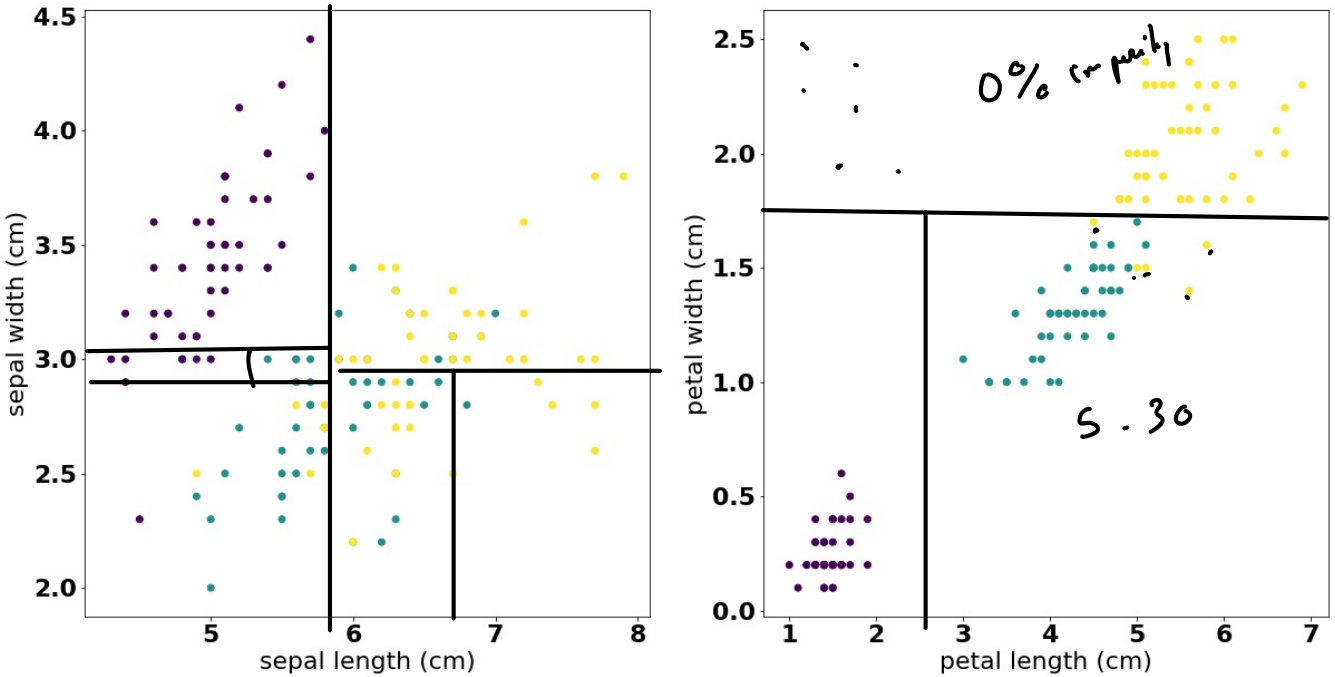
Figure: Iris: setosa, versiocolor, virginica

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

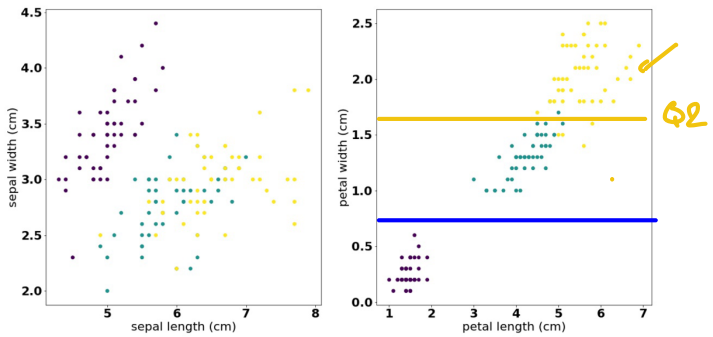
`https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html`

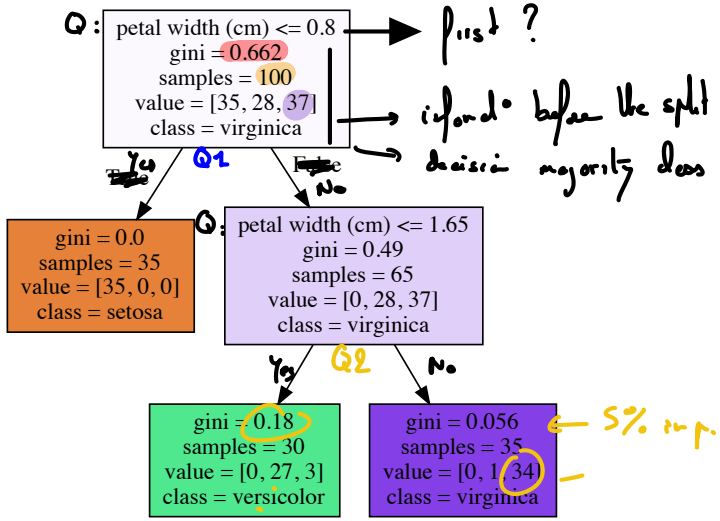
Example: Iris Dataset

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
from sklearn.model_selection import train_test_split
import matplotlib.pyplot as plt

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

#Load the dataset
iris = load_iris()
X_fit, X_val, y_fit, y_val = train_test_split(
    iris.data, iris.target, test_size=0.33, random_state=43)

# Fit the model
clf.fit(X_fit,y_fit)

# Plot tree
plt.figure(figsize=(5,4))
plot_tree(clf, feature_names = iris.feature_names,
                class_names=iris.target_names,
                filled = True)
plt.show()
```

Output:





Example:

```
X_test[0,:], iris.target_names[y_test[0]]
```

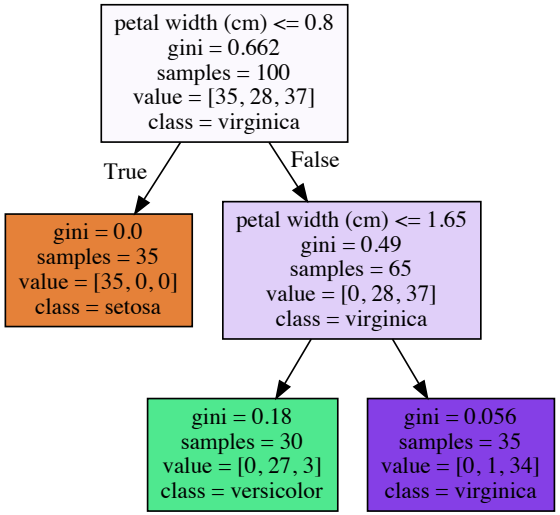
Returns:

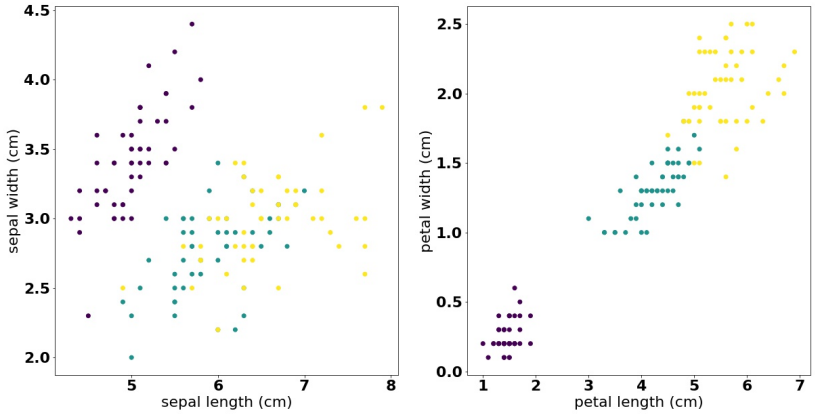
(array([4.8, 3.1, 1.6, 0.2]), 'setosa')

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

Example: Iris Dataset

Output:





Example:

```
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

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

Wooclap time!

1 Allez sur wooclap.com

2 Entrez le code d'événement dans le bandeau supérieur

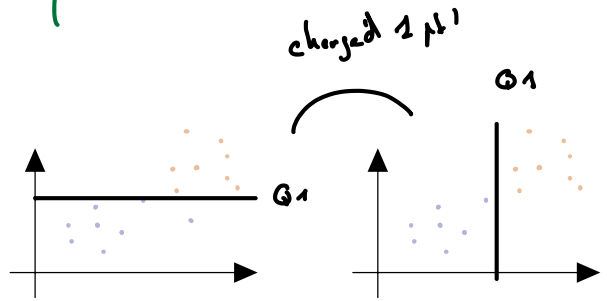
Code d'événement
TAMXAU

1 Envoyez @TAMXAU au 06 44 60 96 62

2 Vous pouvez participer

Désactiver les réponses par SMS

1. The depth is "learned" in DT : nope its a hyperparameter
2. The depth is a hyperparameter ✓ (yes!)
3. I use the validation set to find hyperparameters always : not true for DT
4. There is no train set for Decision Trees yes.

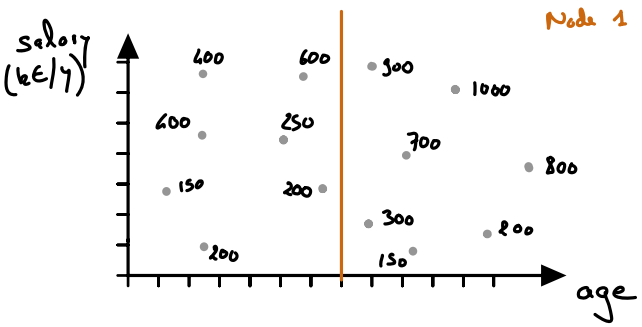


Which of the following statements are true about Decision Trees?

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) * yes!

4 : Work well for high n ✓
→ only few split is proportion

5 : Do not for regress°. ✗
yes they do



Node 1 :

300
1000
700
800
200
300
150

↳ Variance / Dispersion

$$\frac{1}{n}\sum_{i=1}^{7}(x_i - \bar{x})^2$$

~~purity~~

Variance

400
600
250
400
200
150
200

→ Variance

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

1. The same feature cannot be used twice consecutively" → X

yes it can but w. ≠ thresholds.

2. The same feature cannot be used twice overall" → X

3. I can use a pair of features if it gives me a better split

↪ X

4. I want to find the split that has minimal impurity

5. To define a new split, I only use one example

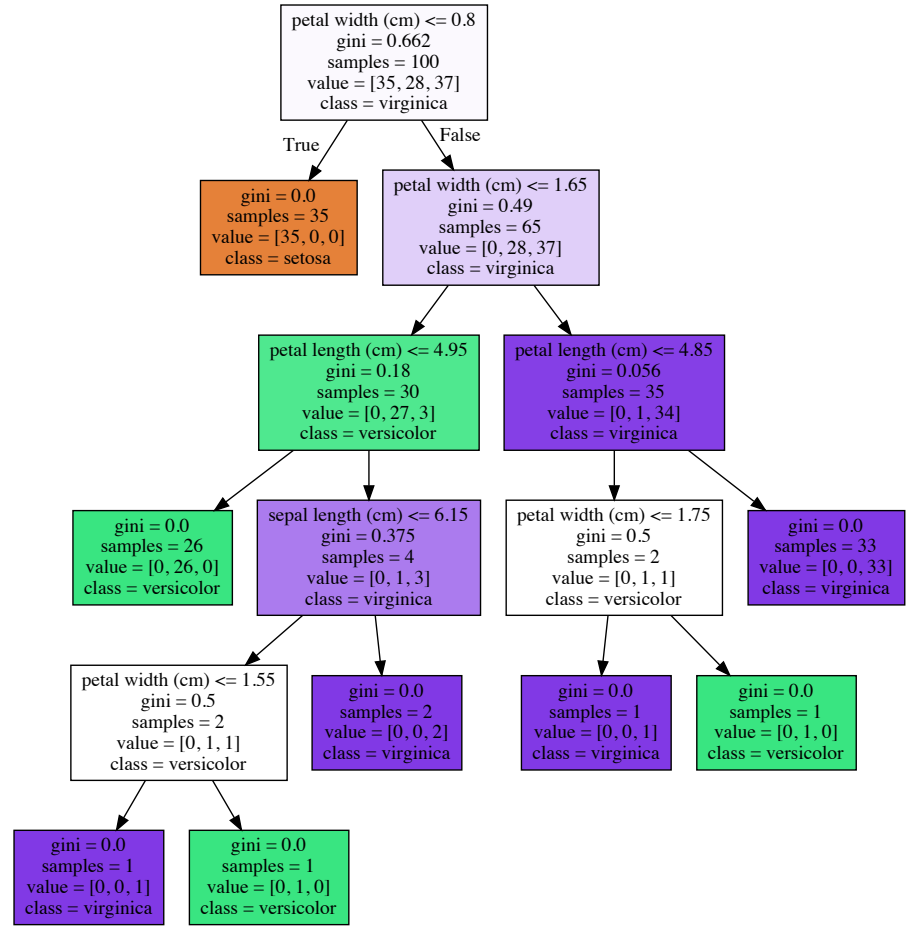
observation

all obs

1 feature

Deeper trees

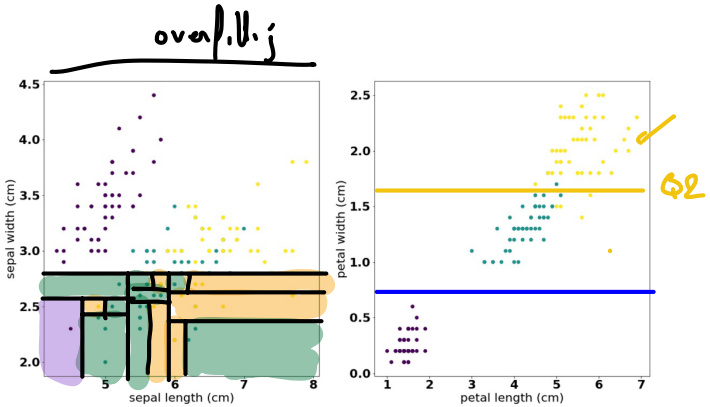
```
# Choose the Learning algorithm
clf = DecisionTreeClassifier(random_state=0)
```



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

Stopping / Pruning

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

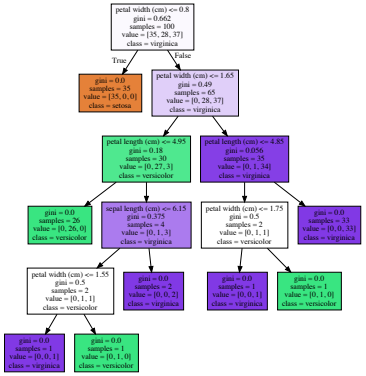


To avoid this problem, we can reduce the complexity of the trees:

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

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

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.

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

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 ?

ideas: inside a tree | errors
uncertainty

→ change dataset
Sol 1 → subsampling → bootstrapping
→ change how we cut.
→ sampling the questions I can check.

Sol° 2: only "try" a certain nb of features for each question. e.g., for Q1 only X_1, X_n can be used

Speed	DT is superior
Interpret	DT - —
Accuracy	Rf is superior

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 ?

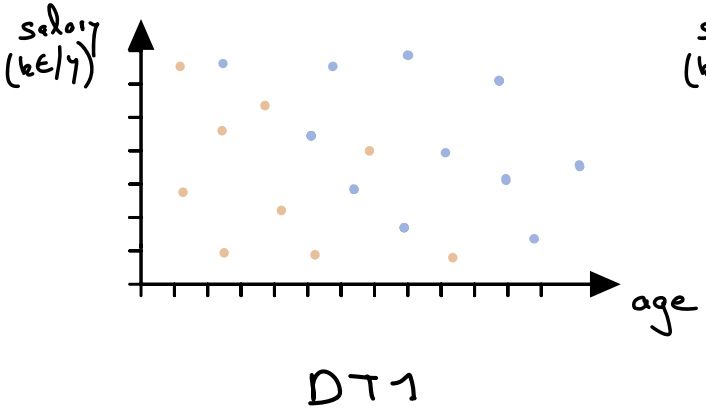
- Instead of the most important features, search the best feature among a random subset (ntry).
- Work on subsets of data (bootstrap=True).
- More `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestRegressor.html`

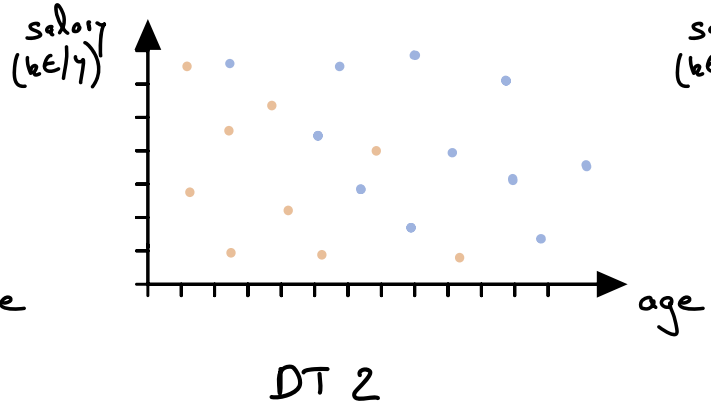
```
# Creating and fitting a Random Forest
from sklearn.ensemble import RandomForestClassifier

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

clf.fit(X_train,y_train)
```

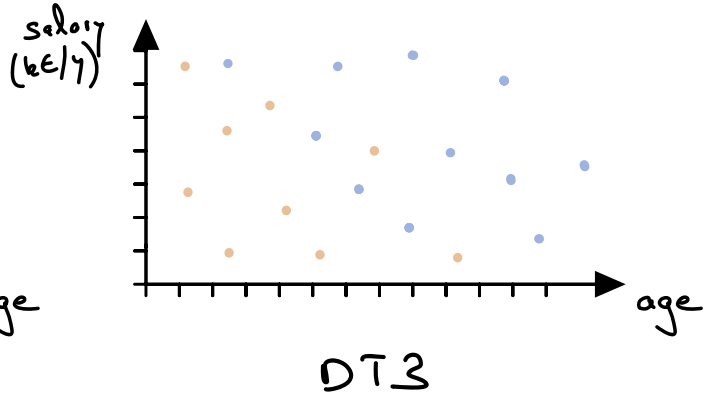
How to aggregate ? How to interpret a Random Forest ?

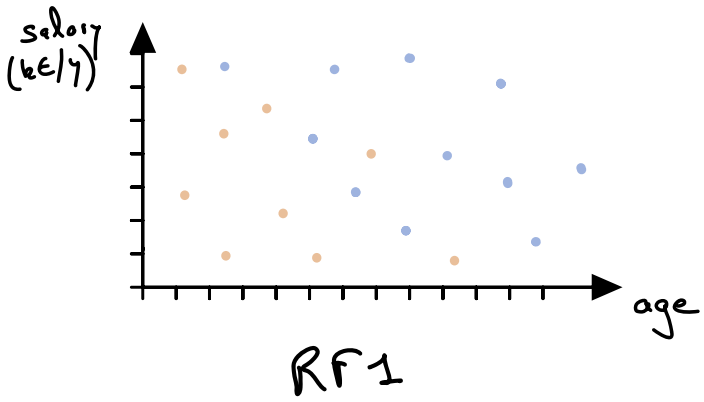
Aggregation

We using a voting or averaging process !





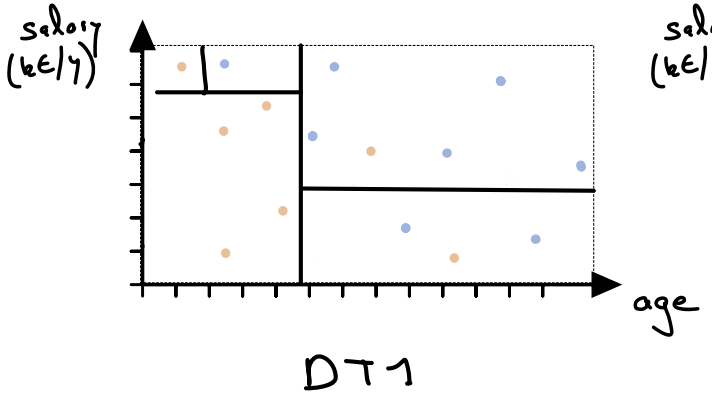


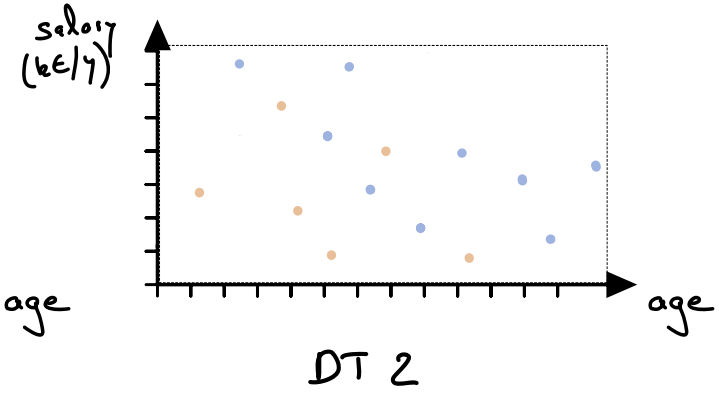


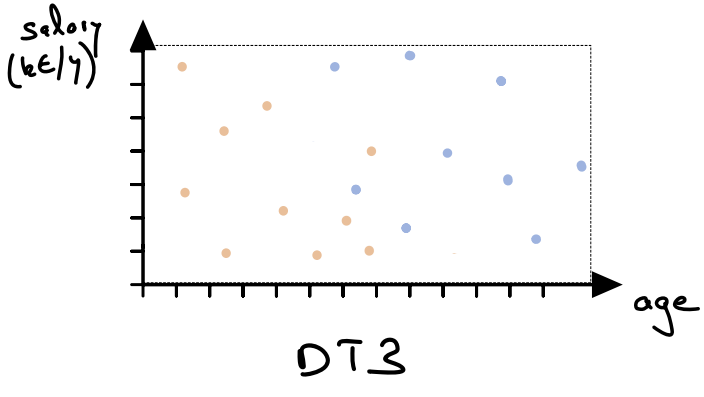
Aggregation

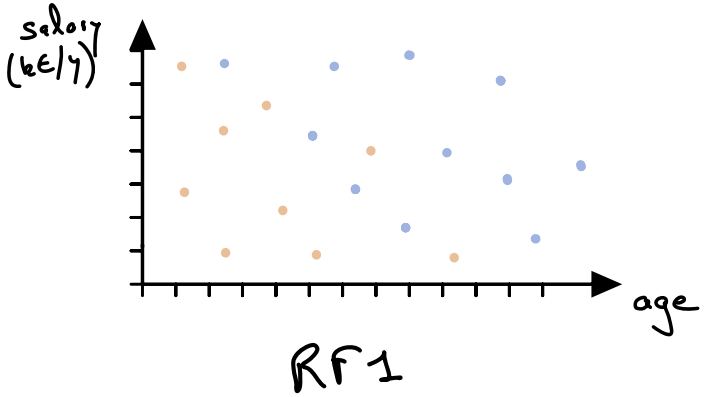
on each, keep 50% of the pairs

We using a voting or averaging process !



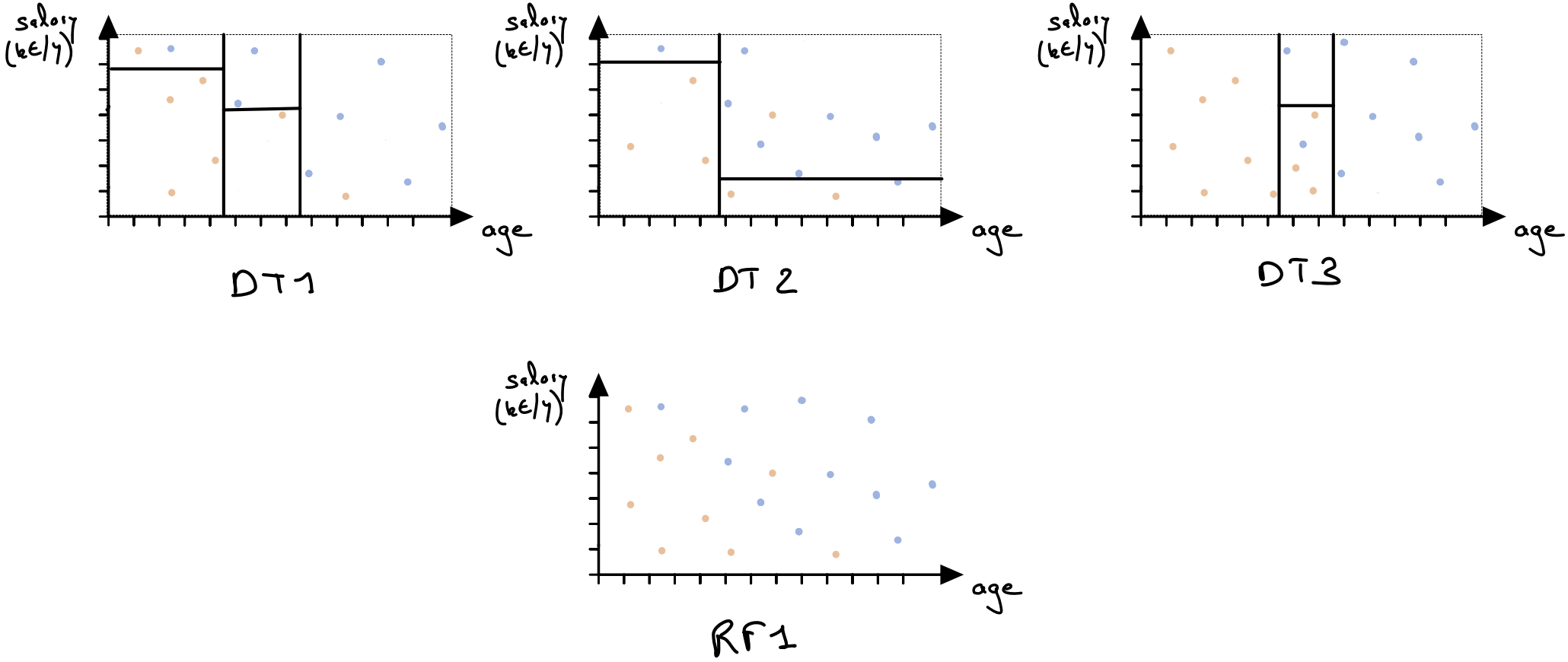






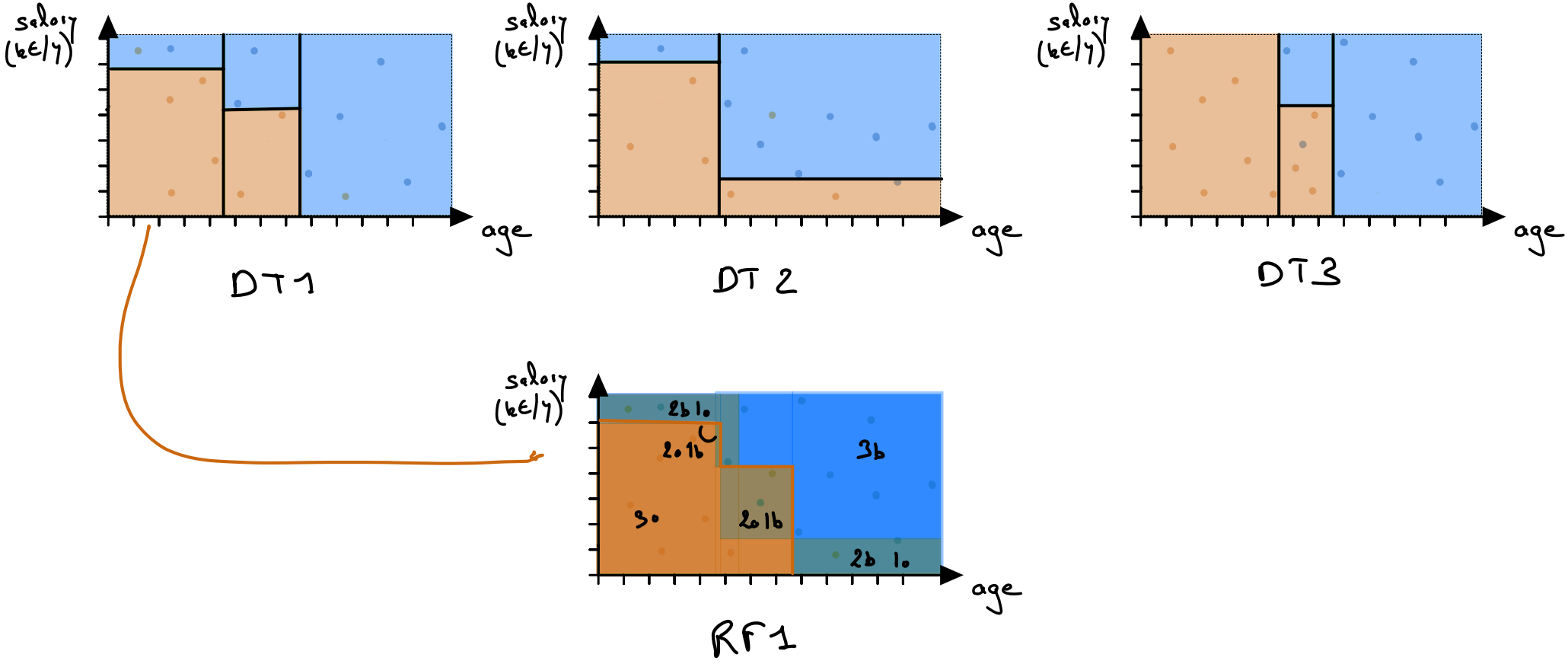
Aggregation

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.

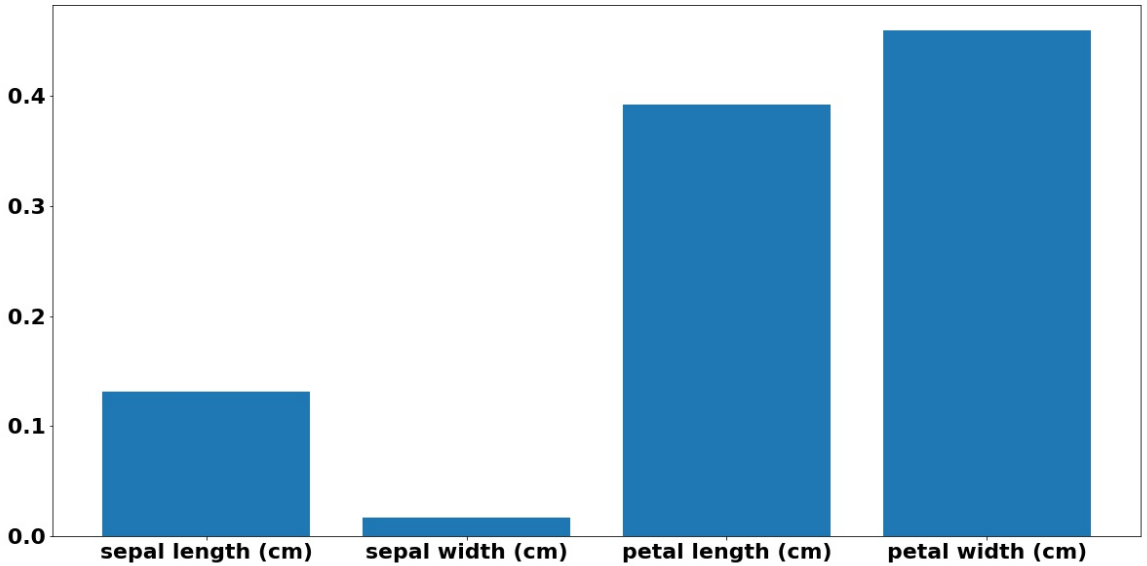


Figure: Feature importane output for a Random Forest Classifier in Python

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

   as much as you can
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

Gaël Varoquaux

Why do tree based models outperform DL on tabular data

2022 at. 1690

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 ?

↪ all the same

aggregate is by averaging

Questions?

Boosting

often even better than RF

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

↳ slower to train because you cannot train independently.

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.