

ML, Decision Trees and Random Forests

Data science Certificate

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April 2025

1 Introduction to Supervised Learning

2 Decision Trees

3 Random Forests

Outline

1 Introduction to Supervised Learning

2 Decision Trees

3 Random Forests

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

- 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



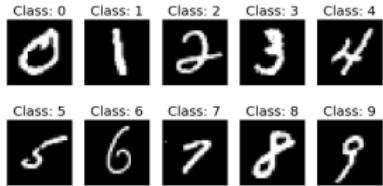
Figure: Iris: setosa, versicolor, virginica

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

Iris Dataset:

- 3 classes : `['setosa', 'versicolor', 'virginica']`
→ $Y \in \{0, 1, 2\}$ encoding each class.
- 50 points per class
→ $n = 150$
- 4 features: `['sepal length', 'sepal width', 'petal length', 'petal width']`
 $X \in \mathbb{R}^4$, → $d = 4$

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 :

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

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

$$n = 60000$$

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

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

Summary of those three datasets

Iris

MNIST

House price prediction

Number of examples n

Number of the features d

Type of the features

Space \mathcal{Y}

Task

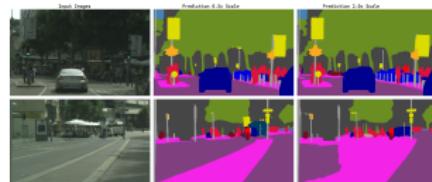
Toy datasets

- In regression:
- In classification:

More examples



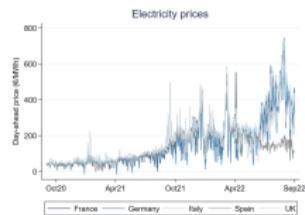
Spam detection



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,
- $Y \in \{0, 1, 2, \dots, K-1\}$ - multi-class classification,
- $Y \in \mathbb{R}$ - regression.

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

Supervised Learning

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

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

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

→ introduce a risk function.

Loss Function

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

Loss function, Generalization Risk and data-dependent predictors

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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): $R(g) = \mathbb{E}[|Y - g(x)|^2]$
- ↪ R is also referred to as *Generalization* risk, or *True* risk.

Loss function, Generalization Risk and data-dependent predictors

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- ↪ R is also referred to as *Generalization* risk, or *True* risk.

⚠ The distribution \mathbb{P} is unknown.

Data-dependent predictors

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

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

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

Supervised Learning: Summary

Supervised Learning: Framework Summary

- Training set: $D_n = \{(x_1, Y_1), \dots, (x_n, Y_n)\}$ (*i.i.d.* $\sim \mathbb{P}$)
- Decision rule (classifier, predictor): $g : \mathcal{X} \rightarrow \mathcal{Y}$
- 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.

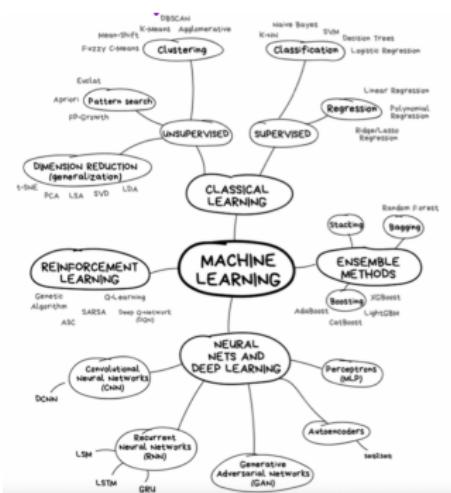


Figure:

Roadmap towards Understanding machine learning!

Training Pipeline

① Fitting

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

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

```
# 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

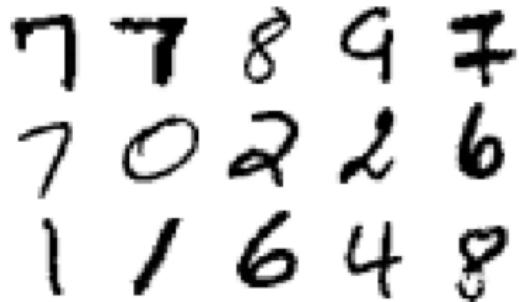


Figure: Digits

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)  
  
+ DecisionTreeClassifier ⓘ ⓘ  
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("Predicted: %d\nTrue: %d" % (predictions[i], y_train.iloc[i]))  
    ax.axis('off')
```

Predicted: 7 Predicted: 7 Predicted: 7 Predicted: 4 Predicted: 7 Predicted: 7 Predicted: 7 Predicted: 7
True: 9 True: 8 True: 1 True: 4 True: 5 True: 5 True: 1 True: 0



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

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

```
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)
```

```
+ LogisticRegression ⓘ ⓘ  
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 regression has "  
    f"{100 * log_reg.score(X_fit, y_fit):.2f}% accuracy"  
)
```

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 regression has 100.00% accuracy

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 regression has "  
    f"{100 * log_reg.score(X_val, y_val):.2f}% accuracy"  
)
```

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 regression has 87.57% accuracy

Wooclap time!



Code d'événement
TAMXAU

1 Allez sur wooclap.com

2 Entrez le code d'événement dans le bandeau supérieur

1 Envoyez [@TAMXAU](https://wooclap.com) au
06 44 60 96 62

2 Vous pouvez participer

Désactiver les réponses par SMS

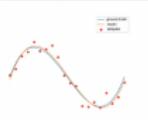
What is true about SML

- | | |
|--|--|
| (1) Supervised Machine Learning does not have inputs | (5) It is necessary to perform well on the train (fit) set for that |
| (2) Supervised Machine Learning can be combined with unsupervised in some contexts | (6) The goal is to predict well on the train (fit) points |
| (3) Supervised Machine Learning does not have outputs | (7) The balance interpretability/speed/performance depends on the method |
| (4) The goal is to predict well on new unseen points | (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...)
```

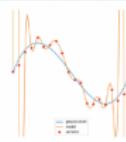
- | |
|---|
| (1) Finding the best parameters of the Forest/Trees |
| (2) Finding the best hyperparameters {n_estimators} |
| (3) Predicting on a test point |



1

A

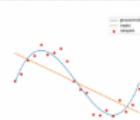
Good fit



2

B

Under-fitting



3

C

Over fitting

Caveat: Overfitting - Toy datasets

- ⚠ The performance on the training set may not reflect the ability to predict on a future point !!
- 💡 Our Goal is to perform well on unseen outputs!!

- 💡 Need to focus on validation/test performance

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

$\mathcal{C} =$

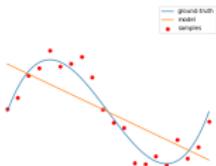
$\hat{R}_n(\theta_n^*)$

$R(\theta_n^*)$

Problem

Dim. of Θ

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



$\mathcal{C} =$ Affine functions

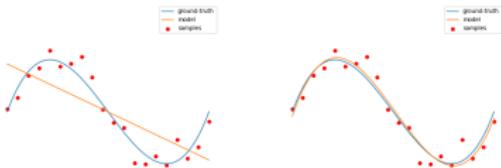
$\hat{R}_n(\theta_n^*)$ high

$R(\theta_n^*)$ high

Problem Underfitting

Dim. of Θ 2

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



$\mathcal{C} =$	Affine functions	$\mathbb{R}_3[X]$
-----------------	------------------	-------------------

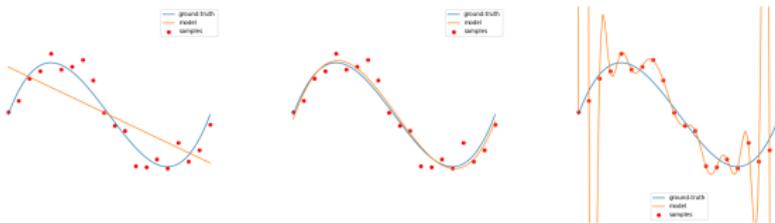
$\hat{R}_n(\theta_n^*)$	high	low
-------------------------	------	-----

$R(\theta_n^*)$	high	low
-----------------	------	-----

Problem	Underfitting	All good
---------	--------------	----------

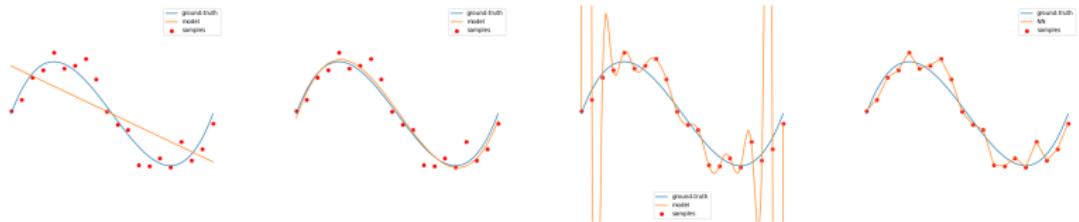
Dim. of Θ	2	4
------------------	---	---

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

- ➊ Training phase
 - ➌ Fitting Phase

- ➋ Validation phase

- ➌ Test phase

- ➍ Deployment

One algorithm to rule SML: Cross validation

💡 Enables to select the best method within multiple methods

```
Entrée [7]: 1 models = {  
2     "Decision Tree": DecisionTreeClassifier(random_state=42),  
3     "Random Forest": RandomForestClassifier(n_estimators=10,random_state=42),  
4     "Logistic Regression": LogisticRegression(multi_class="multinomial", solver="lbfgs", max_iter=100, random_st  
5     "MLP Classifier": MLPClassifier(random_state=42),  
6     "SVM": SVC()  
7 }
```

```
Entrée [12]: 1 cv_results = {}  
2  
3 for name, model in models.items():  
4     kfold = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)  
5     cv_score = cross_val_score(model, X_train, y_train, cv=kfold, scoring="accuracy")  
6     cv_results[name] = cv_score  
7     print(f"\n{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=0.8826785714285714, Std Deviation=0.007804204779790829  
MLP Classifier: Mean CV accuracy=0.8842857142857143, Std Deviation=0.0031237242293813998  
SVM: Mean CV accuracy=0.9505357142857143, Std Deviation=0.005463235193135154
```

```
Entrée [18]: 1 # Convert results to DataFrame for better visualization  
2 results_df = pd.DataFrame(cv_results)  
3 results_df
```

```
Out[18]:
```

	Decision Tree	Random Forest	Logistic Regression	MLP Classifier	SVM
0	0.775893	0.885714	0.880057	0.885714	0.953571
1	0.752679	0.875000	0.860071	0.880143	0.942857
2	0.776788	0.886214	0.883929	0.885714	0.956000
3	0.790179	0.881250	0.865179	0.888393	0.960000
4	0.760714	0.873214	0.879464	0.879464	0.947321

```
Entrée [17]: 1 # Descriptive statistics can also be helpful  
2 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	0.956536
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	0.956000
75%	0.787688	0.885714	0.880057	0.885714	0.965571
max	0.790179	0.886214	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 [1]: 1 from sklearn.model_selection import GridSearchCV
2
3 # Example for SVM
4 param_grid = {
5     'C': [1, 10, 100],
6     'gamma': [0.001, 0.01, 0.1],
7 }
8 grid_search = GridSearchCV(SVC(), param_grid, cv=3, verbose=2)
9 grid_search.fit(X_train_scaled[:10000], y_train[:10000]) # Reduced data size for quicker execution
10
11 print("Best parameters:", grid_search.best_params_)
12 print("Best cross-validation accuracy:", grid_search.best_score_)
13 best_model = grid_search.best_estimator_
14 final_predictions = best_model.predict(X_test_scaled)
15 print("Test set accuracy:", accuracy_score(y_test, final_predictions))
```

```
Entrée [43]: 1 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	mean
0	2.354261	0.049712	1.981289	0.027614	1	0.001	{'C': 1, 'gamma': 0.001}	0.918050	0.930370	0.927663	
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	0.746617	
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	0.746617	
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:

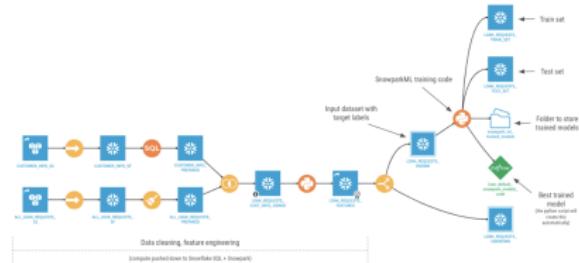


Figure: Dataiku

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

SML -Summary

① Key concepts

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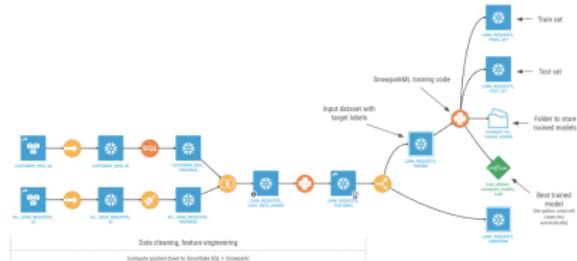


Figure: Dataiku

<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!



Code d'événement
TAMXAU

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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

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
- ③ Find the best hyperparameters in terms of validation error
- ④ Fit the model
- ⑤ Find the best parameters in terms of validation error

```
Entrée [7]: 1 models = [
2     "Decision Tree": DecisionTreeClassifier(random_state=42),
3     "Random Forest": RandomForestClassifier(n_estimators=10,random_state=42),
4     "Logistic Regression": LogisticRegression(multi_class="multinomial", solver="lbfgs", max_iter=100, random_
5     "MLP Classifier": MLPClassifier(random_state=42),
6     "SVM": SVC()
7 ]
```

```
Entrée [12]: 1 cv_results = {}
2
3     for name, model in models.items():
4         kfold = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)
5         cv_score = cross_val_score(model, X_train, y_train, cv=kfold, scoring="accuracy")
6         cv_results[name] = cv_score
7     print(f"\n{name}: Mean CV accuracy={np.mean(cv_scores)}, Std Deviation={np.std(cv_scores)}")
```

Decision Tree: Mean CV accuracy=0.77125, Std Deviation=0.013453124957091512
 Random Forest: Mean CV accuracy=0.8826785714285714, Std Deviation=0.0089570097288568329
 Logistic Regression: Mean CV accuracy=0.875, Std Deviation=0.00784204779798029
 MLP Classifier: Mean CV accuracy=0.8842857142857143, Std Deviation=0.0031237242293813998
 SVM: Mean CV accuracy=0.9585357142857143, Std Deviation=0.005463235193135154

```
Entrée [10]: 1 # Convert results to DataFrame for better visualization
2 results_df = pd.DataFrame(cv_results)
3 results_df
```

	Decision Tree	Random Forest	Logistic Regression	MLP Classifier	SVM
0	0.775693	0.885714	0.882057	0.885714	0.953671
1	0.752679	0.875000	0.865071	0.882143	0.940857
2	0.776766	0.898214	0.883929	0.885714	0.958629
3	0.790179	0.881250	0.865179	0.886393	0.950000
4	0.780714	0.873214	0.875464	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, splitting 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

Reminder on Linear and Logistic regression - towards DT

Limits of Linear and logistic regression - towards DT

Outline

1 Introduction to Supervised Learning

2 Decision Trees

3 Random Forests

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 —> allow complex dependencies.

Decision Tree

Goals of Decision Trees

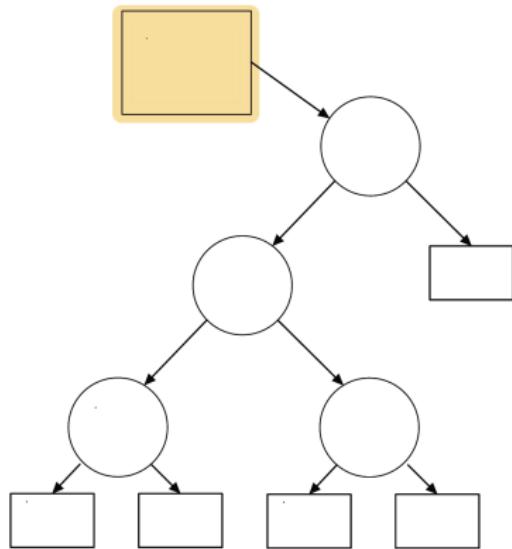
- ① Supervised Learning: solve the classification or regression task
- ② Provide some understanding: what on this example allows me to classify it? What are the important features ?
- ③ Go beyond linear functions —> allow complex dependencies.

Two questions:

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

Inference Phase

- Root = observation = input
- Nodes = tests
- Branches = possible outcomes
- Leaves = final decision = output



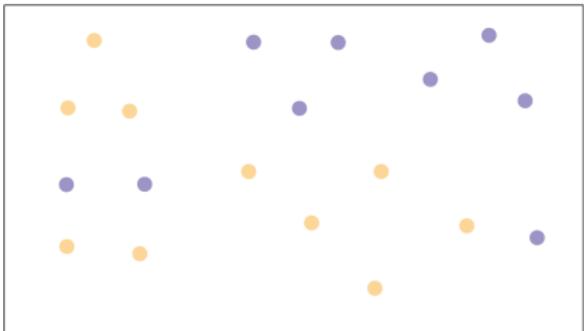
Training: how to build a tree.

Key question !

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

What do you think?

Building trees : CART



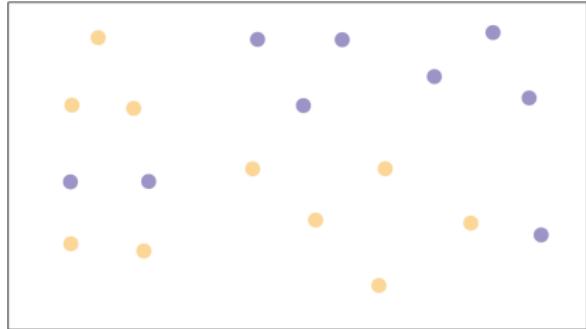
Building trees : CART



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..

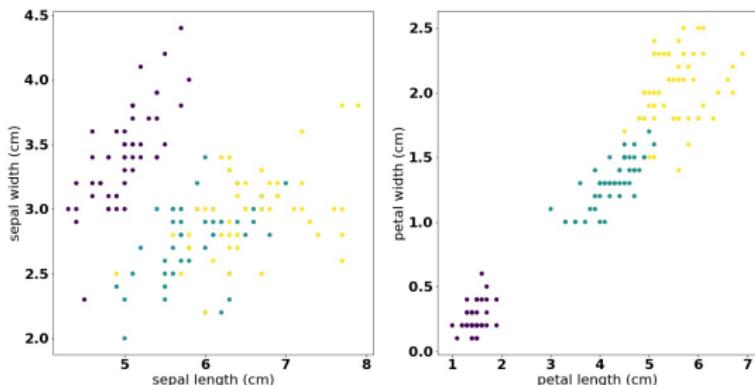
Example: Iris Dataset



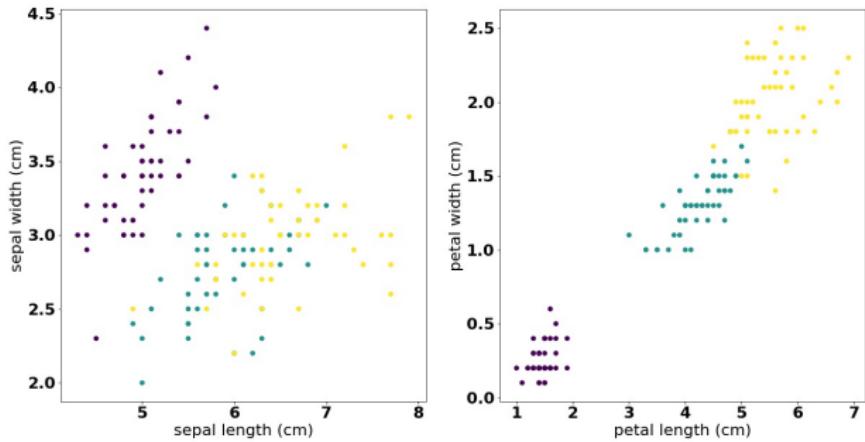
Figure: Iris: setosa, versicolor, virginica

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 practice : 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 ?

```
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

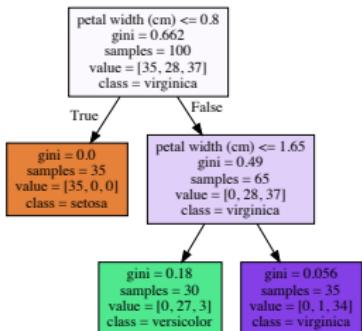
# Choose the Learning algorithm
clf = DecisionTreeClassifier(max_depth = 2)

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

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

# 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]]
```

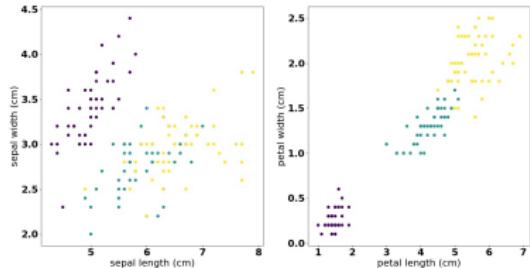
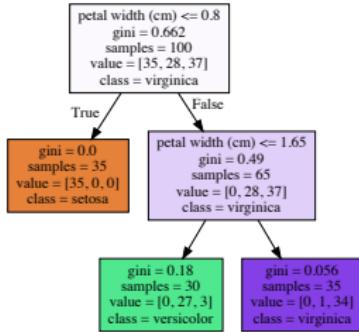
Returns:

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

Code: <https://colab.research.google.com/drive/1dXYIjacNAeASgl54vIWjMqlfgigSVA?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!



Code d'événement
TAMXAU

1 Allez sur wooclap.com

2 Entrez le code d'événement dans le bandeau supérieur

1 Envoyez [@TAMXAU](https://wooclap.com) au
06 44 60 96 62

2 Vous pouvez participer

Désactiver les réponses par SMS

1

The depth is "learned" in DT

2

The depth is a hyperparameter

3

I use the validation set to find hyperparameters

4

There is no train set for Decision Trees

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)

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

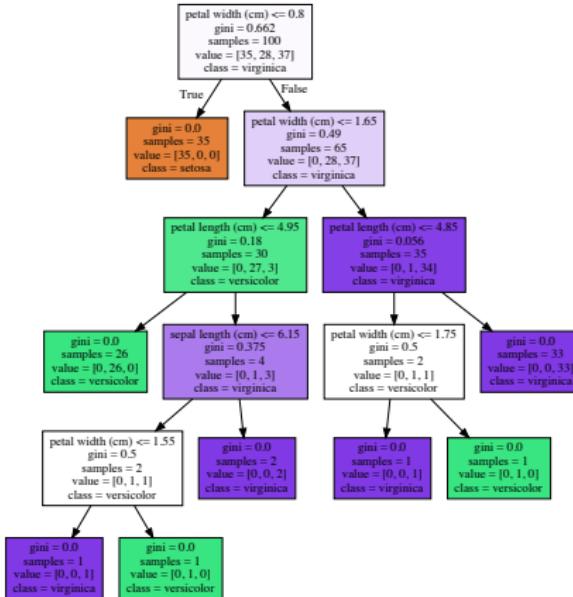
4 I want to find the split that has minimal impurity

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

Deeper trees

```
# Choose the Learning algorithm
```

```
clf = DecisionTreeClassifier(random_state=0)
```



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

Stopping / Pruning

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

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

① Stopping rules

- ▶ Set a minimum number of samples inside each leaf.
- ▶ Set a maximum depth.

② Pruning

- ▶ Reduced error pruning.
- ▶ Cost complexity pruning.

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, interpret, 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

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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 !

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.

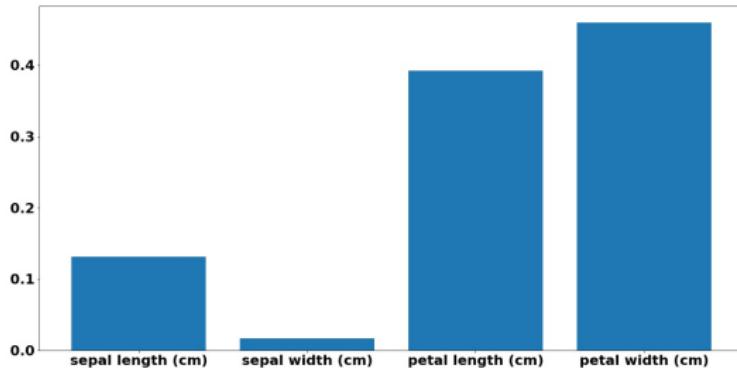


Figure: Feature importance output for a Random Forest Classifier in Python

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 ?

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.

Face completion with multi-output estimators



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

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

Lab :

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

