Decision Trees and Random Forests
Data science Certificate

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Outline

A Reminder on Supervised Learning

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

3 Examples:

- Iris Dataset:
- MNIST:
- House price prediction

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']*

Example: MNIST Dataset

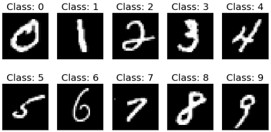

Figure:

Digit recognition from an image:

- 10 classes : $Y_i \in$
- 60k images, (50k train, 10k test), balanced
- 784 features.

House price Prediction

- Output : house value $Y \in$
- 1500 examples
- 81 features: Construction year, Neighborhood, Surface, Floor, Balcony: both quantitative and qualitative, some ordinal variables.

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			

Learning Pipeline

1. Training phase

2. Validation phase

3. Test phase

4. Deployment

Reminder on Linear and Logistic regression

Limits of Linear and logistic regression

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 ?

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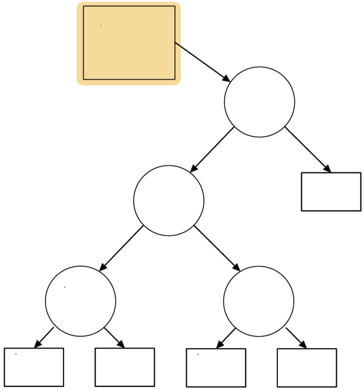
Two questions:

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

Inference Phase

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



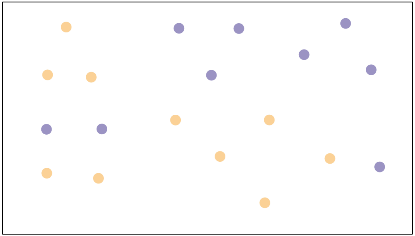
Training: how to build a tree.

Key question !

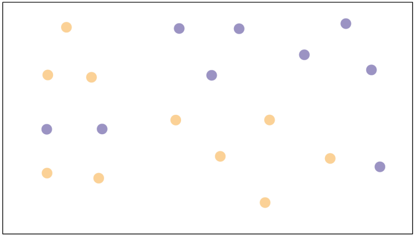
- What is a good tree?
- What do I need to choose?
- How to choose?

What do you think?

Building trees : CART



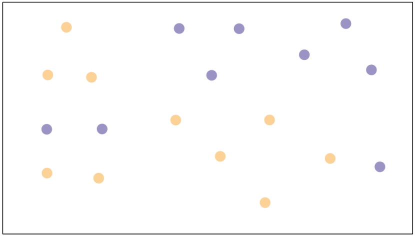
Building trees : CART



How to chose the best cut ?

- e.g., Given a possible cut, measure the reduction of ńăimpurityăż:
  - 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**.

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

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

Example: Iris Dataset

Figure: Iris: setosa, versiocolor, virginica

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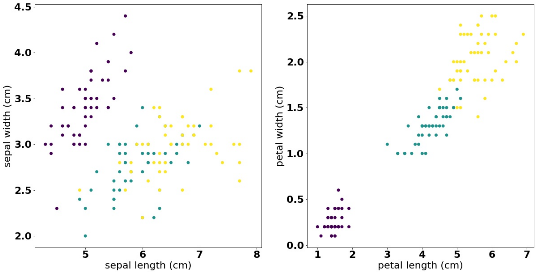
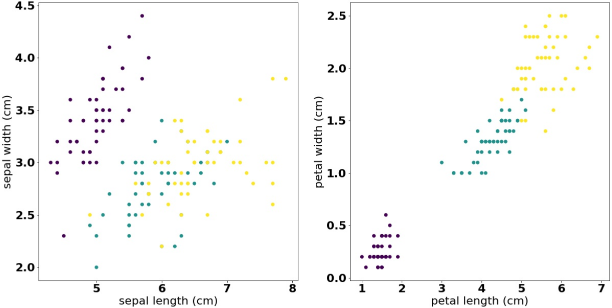


Exercise: Guess Classification tree for Iris Dataset



In pratice : Scikit Learn

Universal Python library for Machine Learning:

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

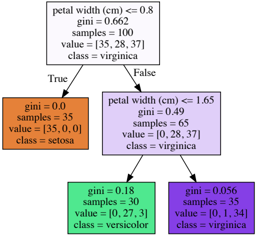
https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html

Example: Iris Dataset

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

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

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

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

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

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

What do we need to specify ?

Output:



Example:

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

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

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

Example: Iris Dataset

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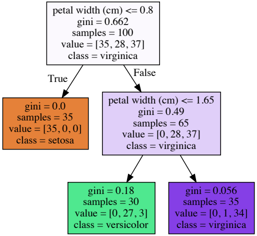

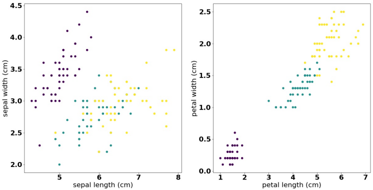

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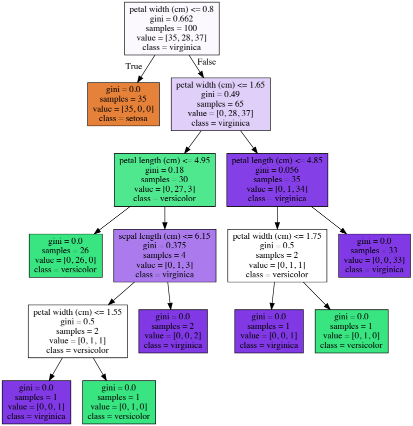
What if I use a deeper tree ? Or if I do not specify the depth in the model definition ?

Deeper trees

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



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

Stopping / Pruning

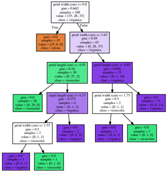
Trees that achieve perfect classification may suffer from over-fitting. (see example in the lab)

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, 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: ńărandom forests builds multiple decision trees and merges them together to get a more accurate and stable predictionsăż.
$\hookrightarrow$key idea: create variable trees + aggregate them

How to create variability ?

Random Forests

To put it in simple words: ńărandom forests builds multiple decision trees and merges them together to get a more accurate and stable predictionsăż.
↬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`

```python
# 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.

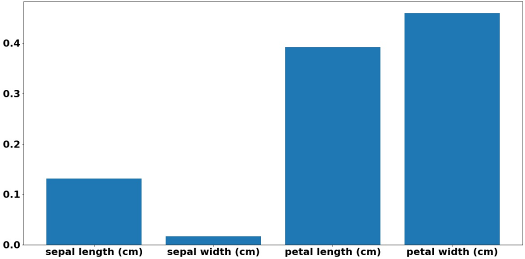


Figure: Feature importane output for a Random Forest Classifier in Python

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. Fast to train but slow to provide new predictions -> ineffective for ńăreal-time predictionsăż.
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.

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.