JAVIER GALEANO, MARZO DE 2022

Notas escépticas sobre el Machine Learning

Lecture 2: Classification Problems

Classification problem in ML

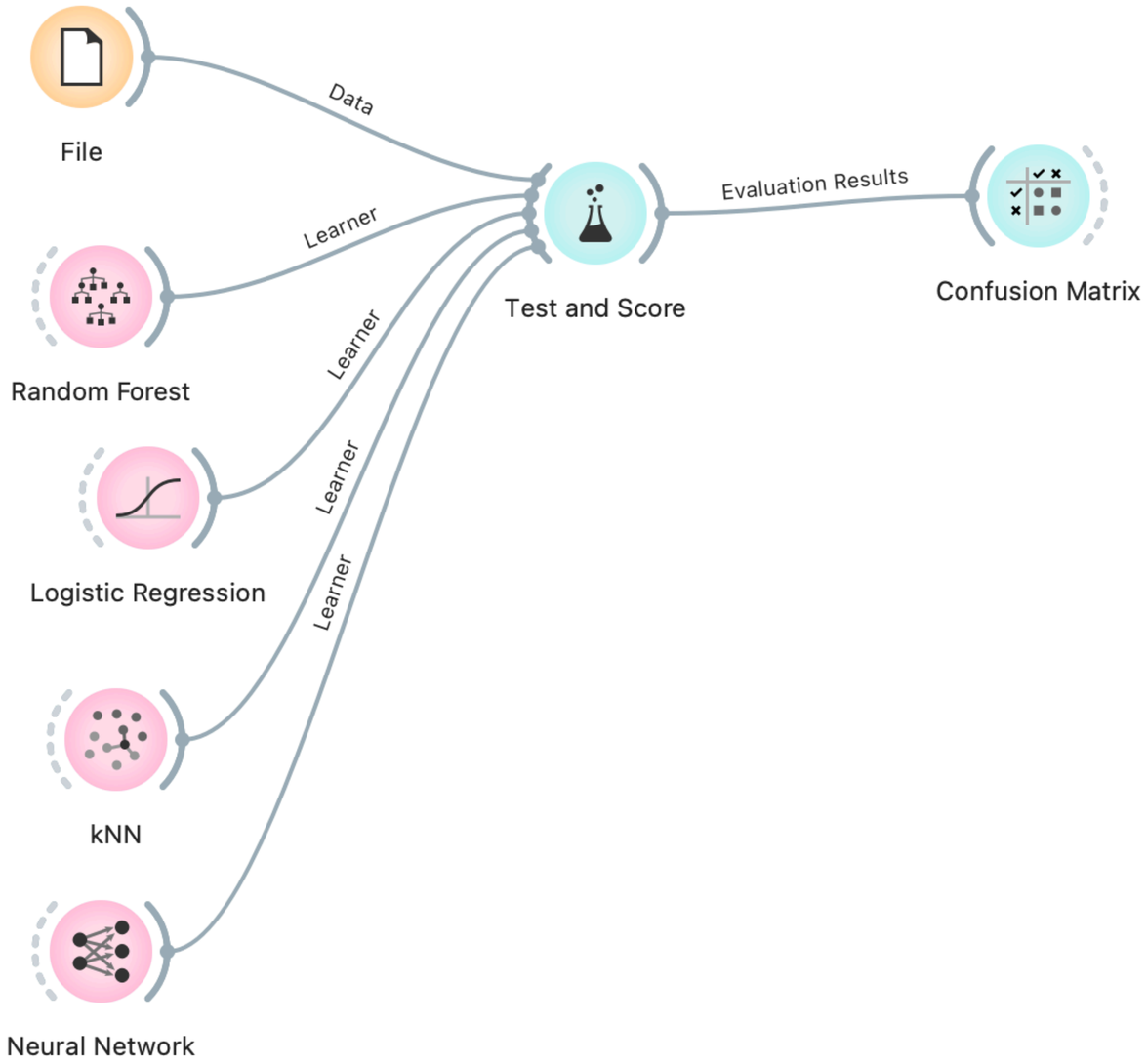
ID	Clump	UnifSize	UnifShape	MargAdh	SingEpiSize	BareNuc	BlandChrom	NormNucl	Mit	Class
1000025	5	1	1	1	2	1	3	1	1	benign
1002945	5	4	4	5	7	10	3	2	1	benign
1015425	3	1	1	1	2	2	3	1	1	malignant
1016277	6	8	8	1	3	4	3	7	1	benign
1017023	4	1	1	3	2	1	3	1	1	benign
1017122	8	10	10	8	7	10		7	1	malignant
1018099	1	1	1	1	2	10	3	1	1	benign
1018561	2	1	2	H	2	1	3	1	1	benign
1033078	2	1	1	1	2	1	1	1	5	benign
1033078	4	2	1	1	2	1	2	1	1	benign

9/03/2022

Classification

In classification, the goal is to predict a *class label*, which is a choice from a predefined list of possibilities.

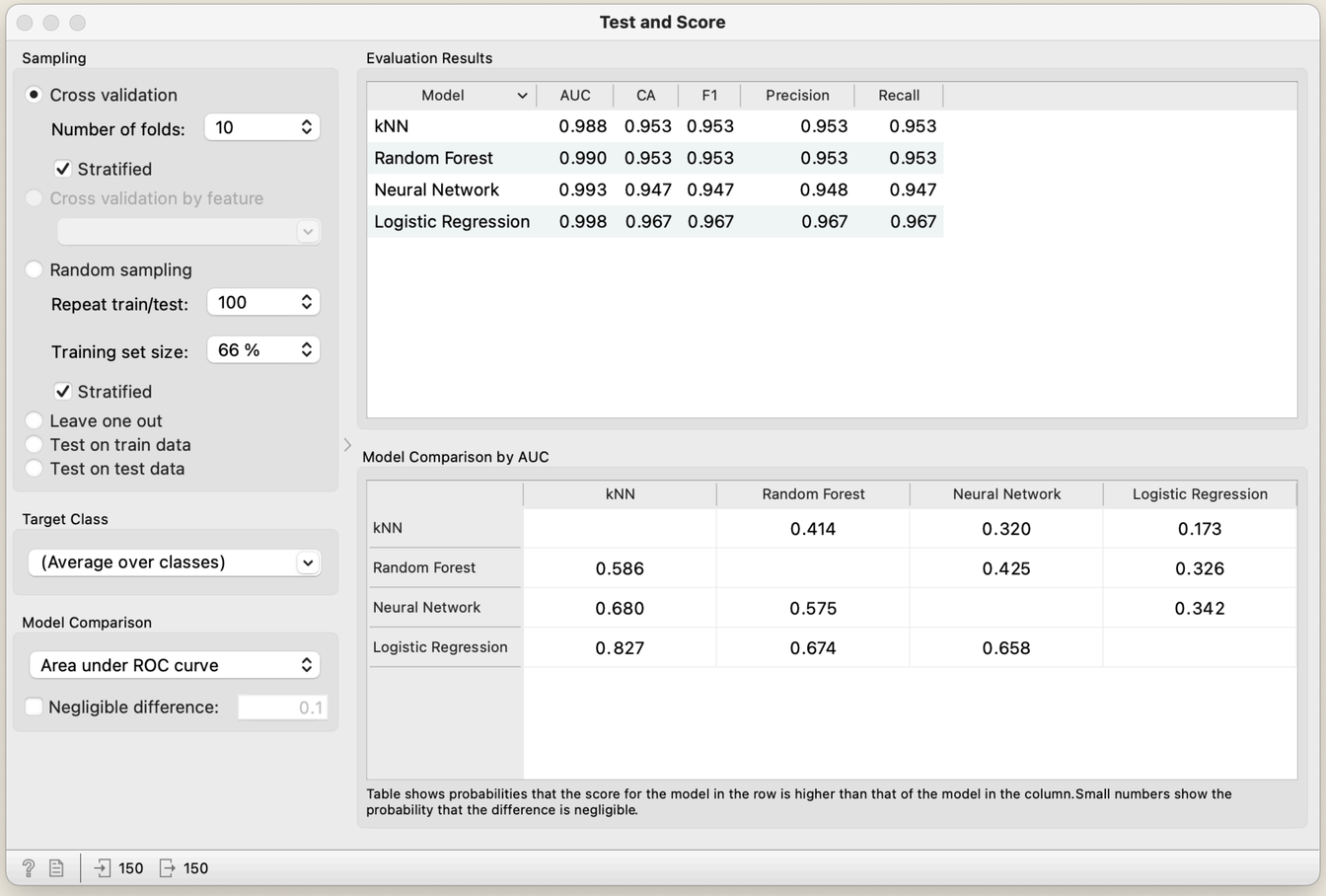
- Binary Classification
- Multiclass Classification



9/MARZO/2022

Scoring

- K-cross validation
- Test & Score
- Confusion Matrix



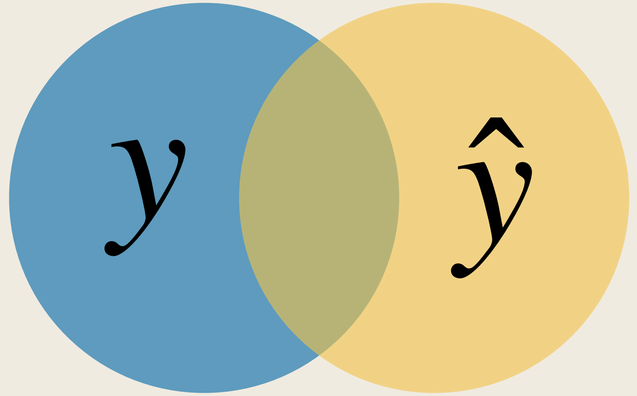
Evaluation metrics in classification

- We are talking about some metrics:
- Jaccard index,
- Confusion matrix

Jaccard index

y = True values (actual values)

$\hat{y}$ = Predicted values of our model



Jaccard index [0,1]

$$J(y,\hat{y}) = \frac{|y \cap \hat{y}|}{|y \cup \hat{y}|} = \frac{|y \cap \hat{y}|}{|y| + |\hat{y}| - |y \cap \hat{y}|}$$

Ejemplo

$y = [0,0,0,0,0,0,1,1,1,1,1]$ $\hat{y} = [1,1,0,0,0,0,0,1,1,1,1,1]$

$$J(y,\hat{y}) = \frac{|y \cap \hat{y}|}{|y| + |\hat{y}| - |y \cap \hat{y}|} = \frac{8}{10 + 10 - 8} = 0.66$$

Confusion Matrix

TP = True Positives

FN = False Negatives

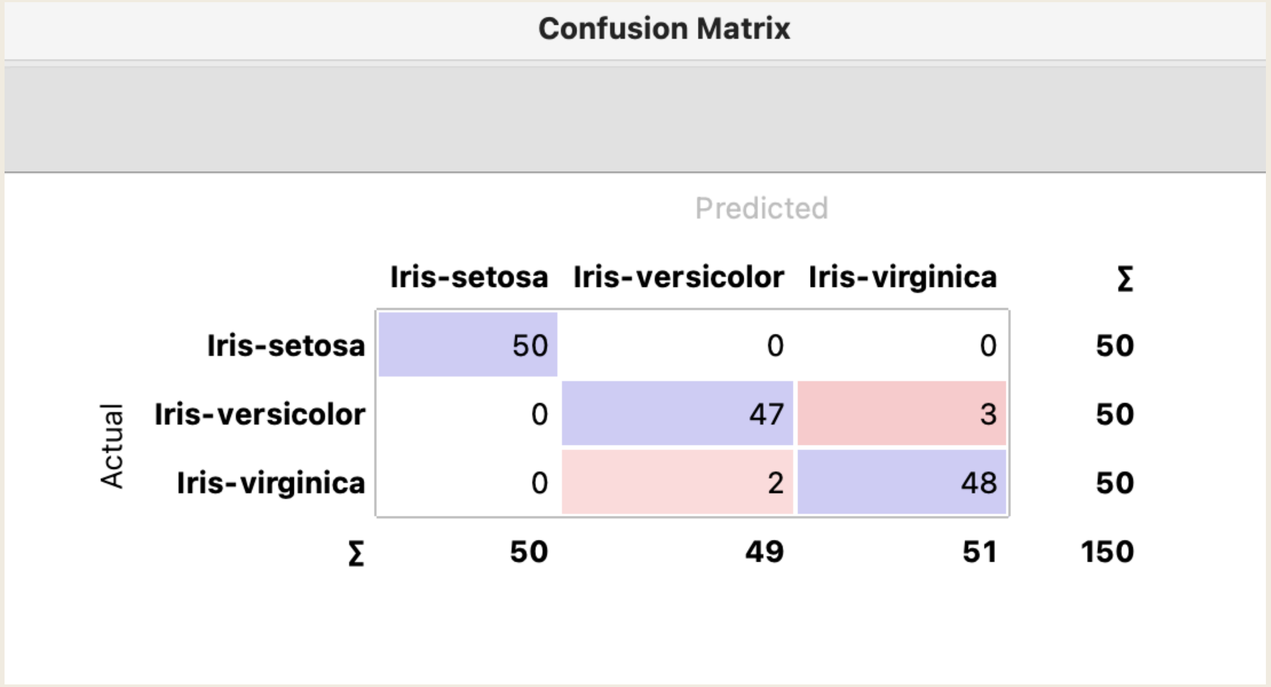
FP = False Positives

TN = True Negatives

$$\textbf{Precision} = \frac{TP}{TP + FP}$$

$$\textbf{Recall} = \frac{TP}{TP + FN}$$

$$\textbf{F1-score}\ [0,1] = \frac{2 * Precision * Recall}{Precision + Recall}$$



Classification Accuracy is the proportion of correctly classified examples

$$CA = \frac{TP}{Total}$$

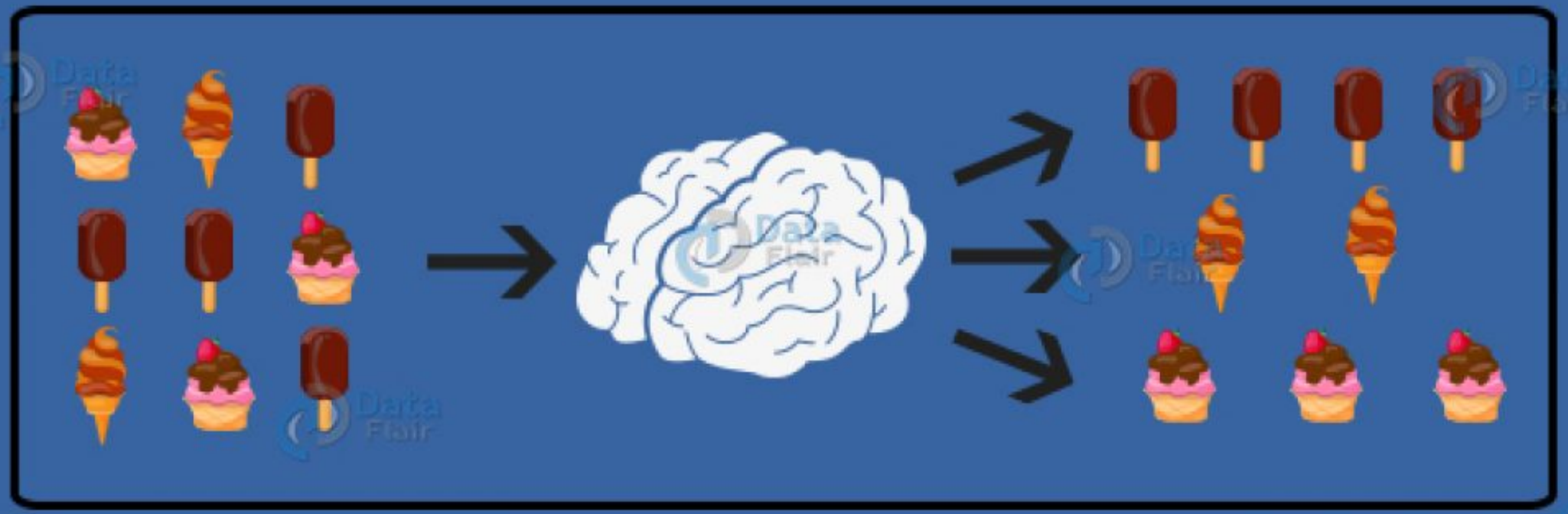
Classification Algorithms

Machine Learning Classification Algorithms

Logistic Regression

Naive Bayes

Decision Tree



Support Vector Machines

Random Forest

K-Nearest Neighbou

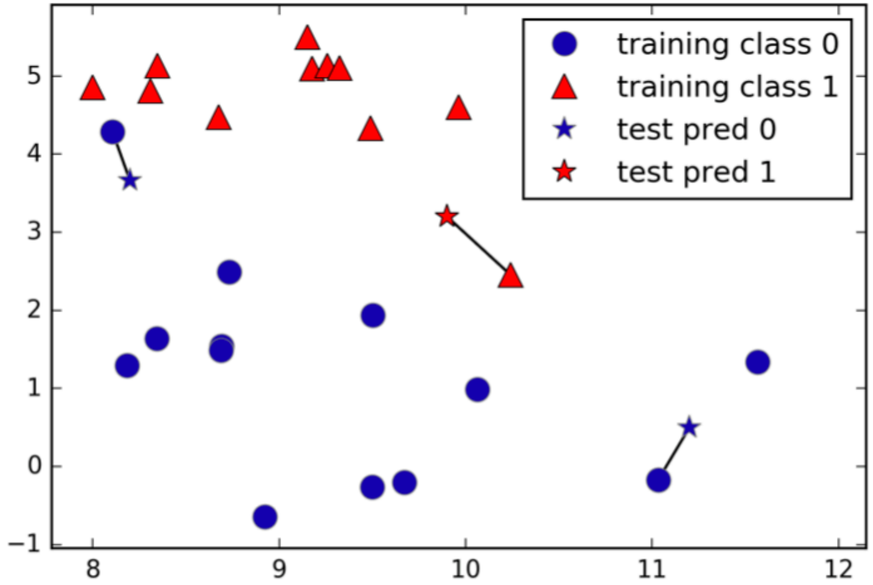


Figure 2-4. Predictions made by the one-nearest-neighbor model on the forge dataset

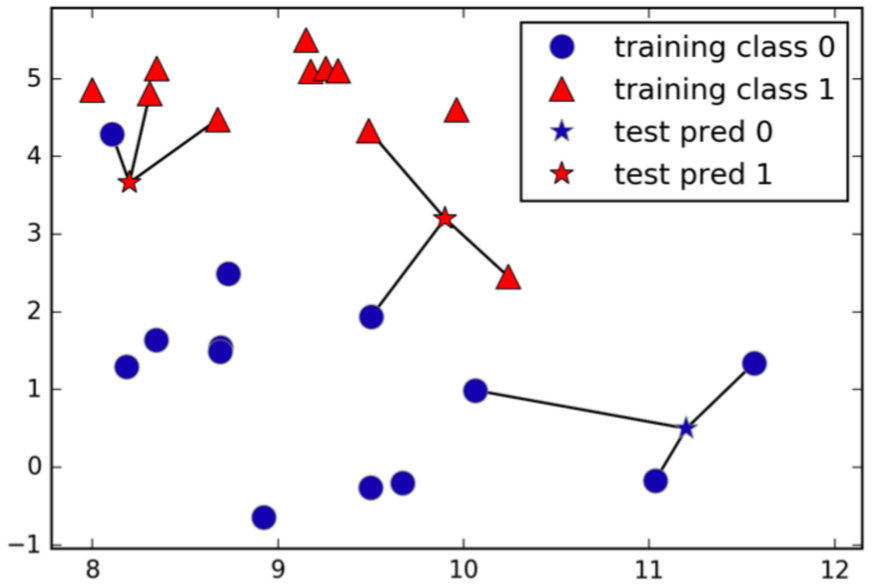
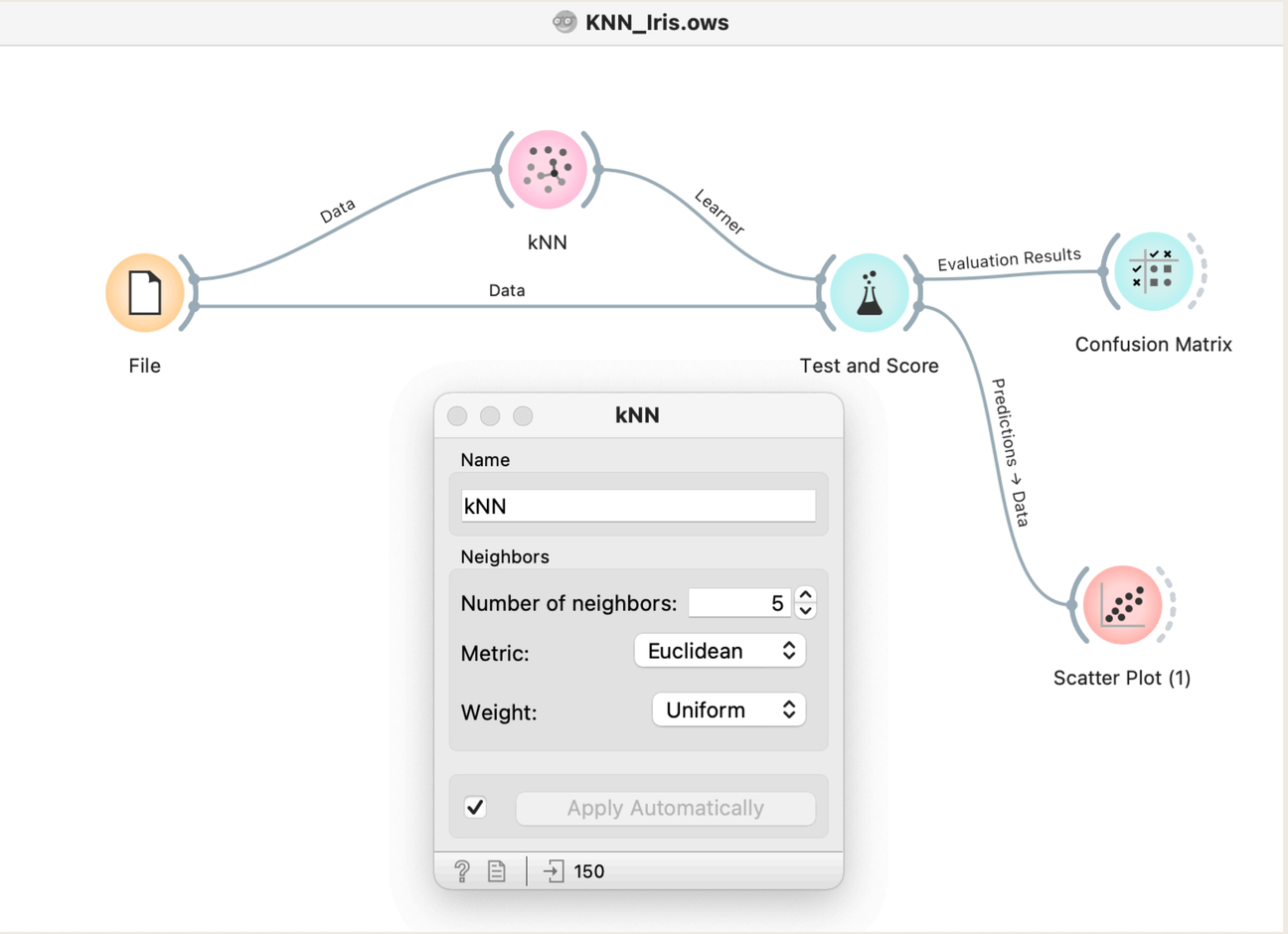


Figure 2-5. Predictions made by the three-nearest-neighbors model on the forge dataset

16/03/2022

K-Nearest Neighbors

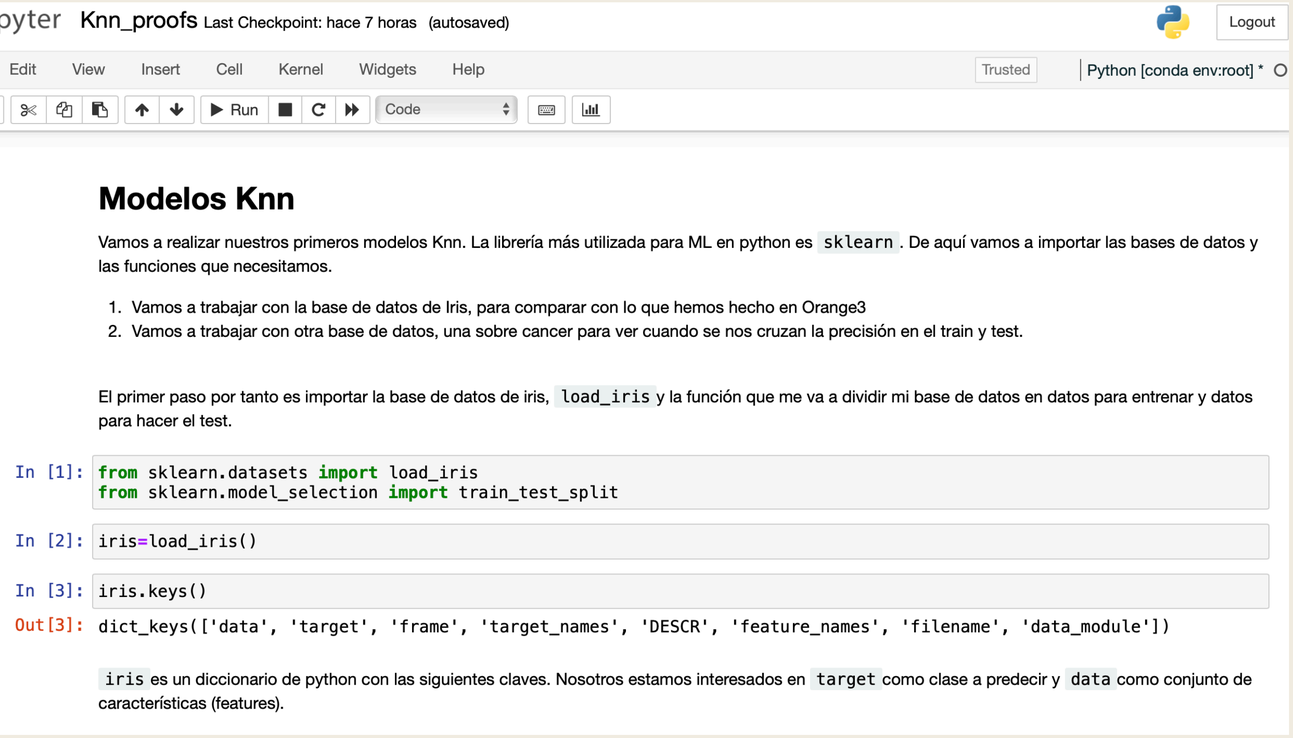
- Building the k-NN algorithm consists only of storing the training dataset.
- To make a prediction for a new data point, the algorithm finds the closest data points in the training dataset—its “nearest neighbors.”



16/MARZO/2022

K-nearest Neighbors

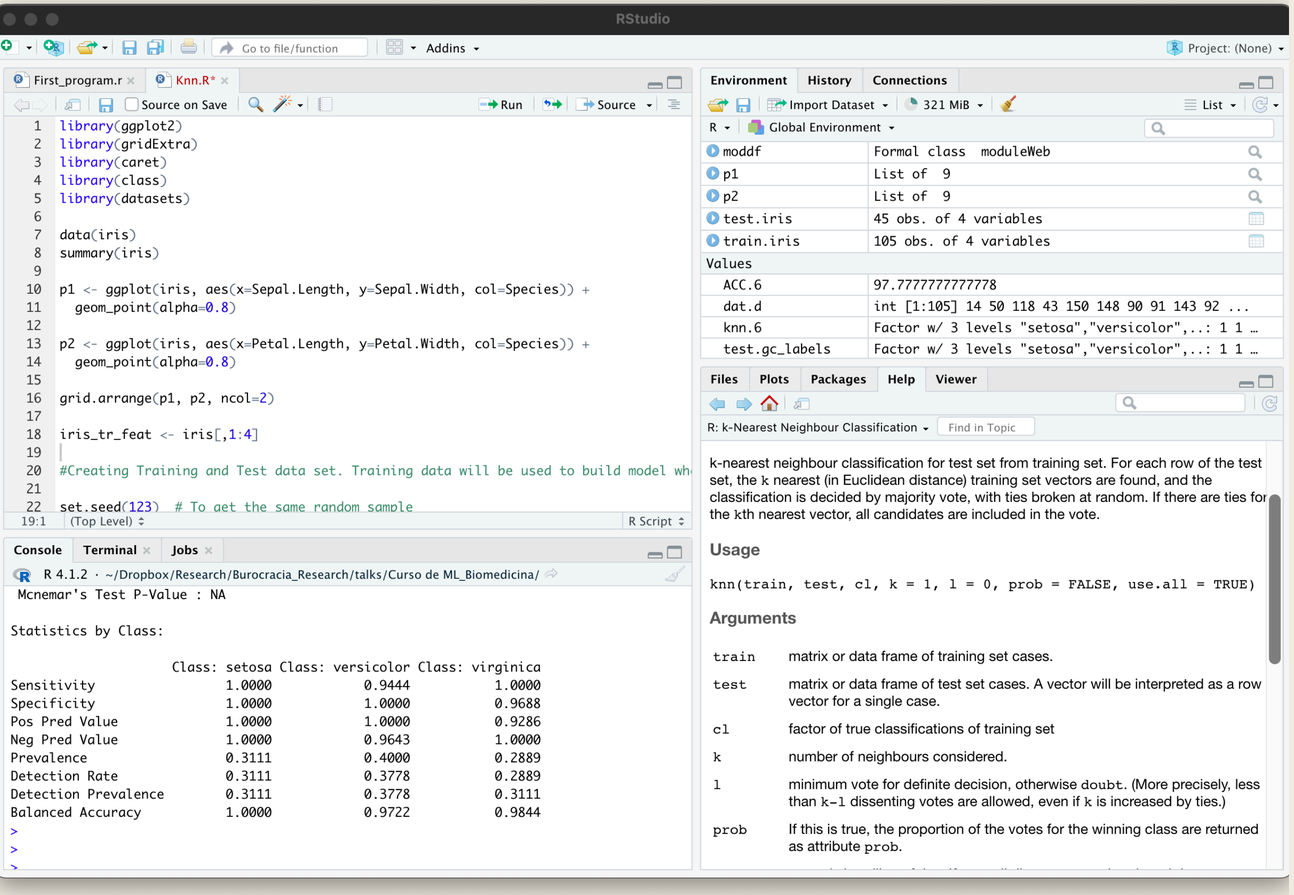
- Iris
- KNN –> Test Score –> Confusion Matrix
- Constant ->Test Score –> Confusion Matrix
- Scatter Plot (KNN)



16/MARZO/2022

K-nearest Neighbors in Python

- Iris
- KNN –> Test Score –> Confusion Matrix



16/MARZO/2022

K-nearest Neighbors in R

- Iris
- KNN –> Test Score –> Confusion Matrix
-

Patient ID	Age	Sex	BP	Cholesterol	Drug
p1	Young	F	High	Normal	Drug A
p2	Young	F	High	High	Drug A
p3	Middle-age	F	Hiigh	Normal	Drug B
p4	Senior	F	Normal	Normal	Drug B
p5	Senior	M	Low	Normal	Drug B
p6	Senior	M	Low	High	Drug A
p7	Middle-age	M	Low	High	Drug B
p8	Young	F	Normal	Normal	Drug A
p9	Young	M	Low	Normal	Drug B
p10	Senior	M	Normal	Normal	Drug B
p11	Young	M	Normal	High	Drug B
p12	Middle-age	F	Normal	High	Drug B
p13	Middle-age	M	High	Normal	Drug B
p14	Senior	F	Normal	High	Drug A
p15	Middle-age	F	Low	Normal	?

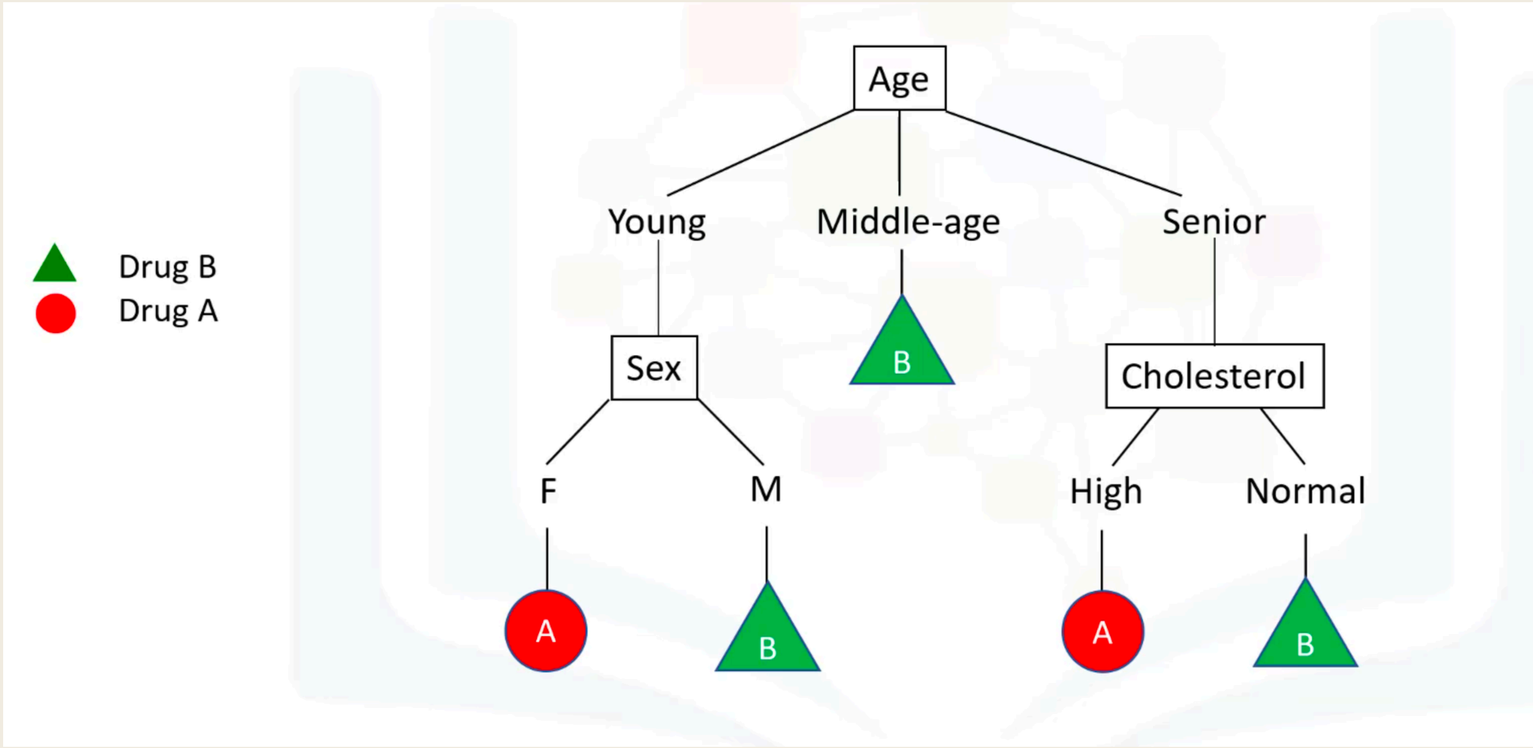
16/MARZO/2022

Decision Tree

- What exactly is a decision tree?

How to build a decision tree?

1. Choose an attribute from your dataset.
2. Calculate the significance of attribute in splitting of data.
3. Split data based on the value of the best attribute.
4. Go to step 1.



How to calculate the significance?

Information gain is the information that can increase the level of certainty after splitting.

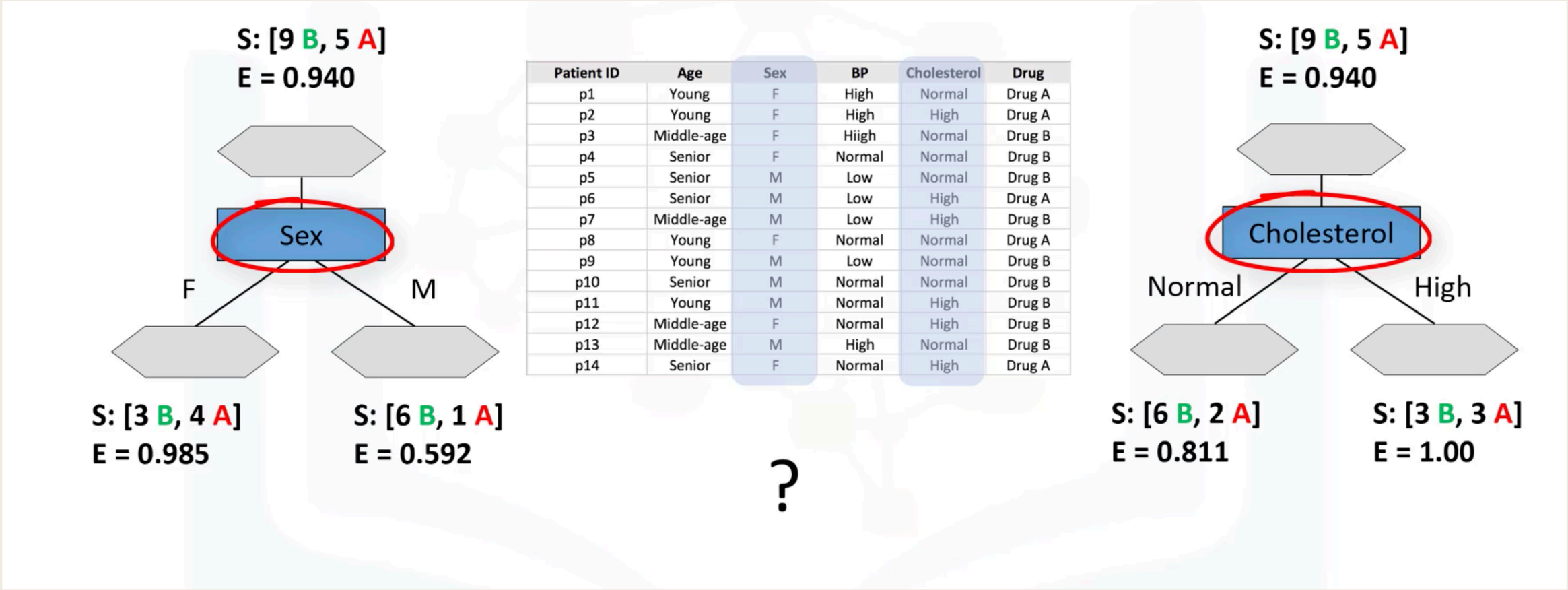
Information Gain = (Entropy before split) – (weighted entropy after split)

In every step, we want to dismiss the impurity of the nodes. Impurity is calculated by Entropy of data in the node

$$E = -\sum_i p_i \log_2(p_i)$$

Entropy is the amount of information disorder. If the samples are completely homogeneous the entropy is zero.

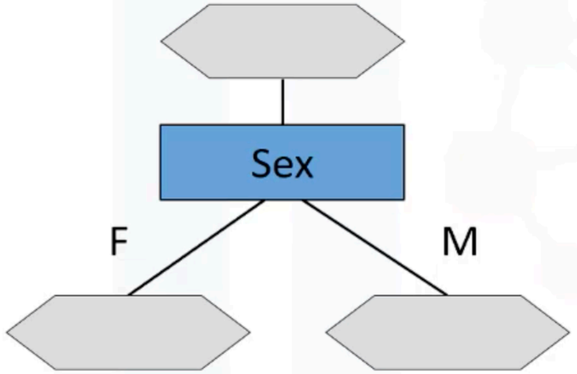
Which attributes is the best?



Patient ID	Age	Sex	BP	Cholesterol	Drug
p1	Young	F	High	Normal	Drug A
p2	Young	F	High	High	Drug A
p3	Middle-age	F	Hiigh	Normal	Drug B
p4	Senior	F	Normal	Normal	Drug B
p5	Senior	M	Low	Normal	Drug B
p6	Senior	M	Low	High	Drug A
p7	Middle-age	M	Low	High	Drug B
p8	Young	F	Normal	Normal	Drug A
p9	Young	M	Low	Normal	Drug B
p10	Senior	M	Normal	Normal	Drug B
p11	Young	M	Normal	High	Drug B
p12	Middle-age	F	Normal	High	Drug B
p13	Middle-age	M	High	Normal	Drug B
p14	Senior	F	Normal	High	Drug A

$$E = -\sum_i p_i \log_2(p_i)$$

S: [9 B, 5 A]
E = 0.940



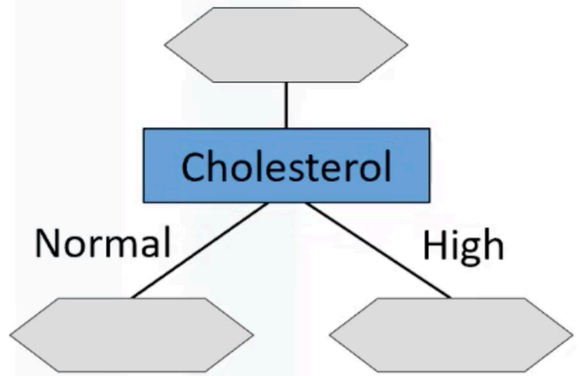
S: [3 B, 4 A]
E = 0.985

S: [6 B, 1 A]
E = 0.592

Patient ID	Age	Sex	BP	Cholesterol	Drug
p1	Young	F	High	Normal	Drug A
p2	Young	F	High	High	Drug A
p3	Middle-age	F	Hiigh	Normal	Drug B
p4	Senior	F	Normal	Normal	Drug B
p5	Senior	M	Low	Normal	Drug B
p6	Senior	M	Low	High	Drug A
p7	Middle-age	M	Low	High	Drug B
p8	Young	F	Normal	Normal	Drug A
p9	Young	M	Low	Normal	Drug B
p10	Senior	M	Normal	Normal	Drug B
p11	Young	M	Normal	High	Drug B
p12	Middle-age	F	Normal	High	Drug B
p13	Middle-age	M	High	Normal	Drug B
p14	Senior	F	Normal	High	Drug A

?

S: [9 B, 5 A]
E = 0.940



S: [6 B, 2 A]
E = 0.811

S: [3 B, 3 A]
E = 1.00

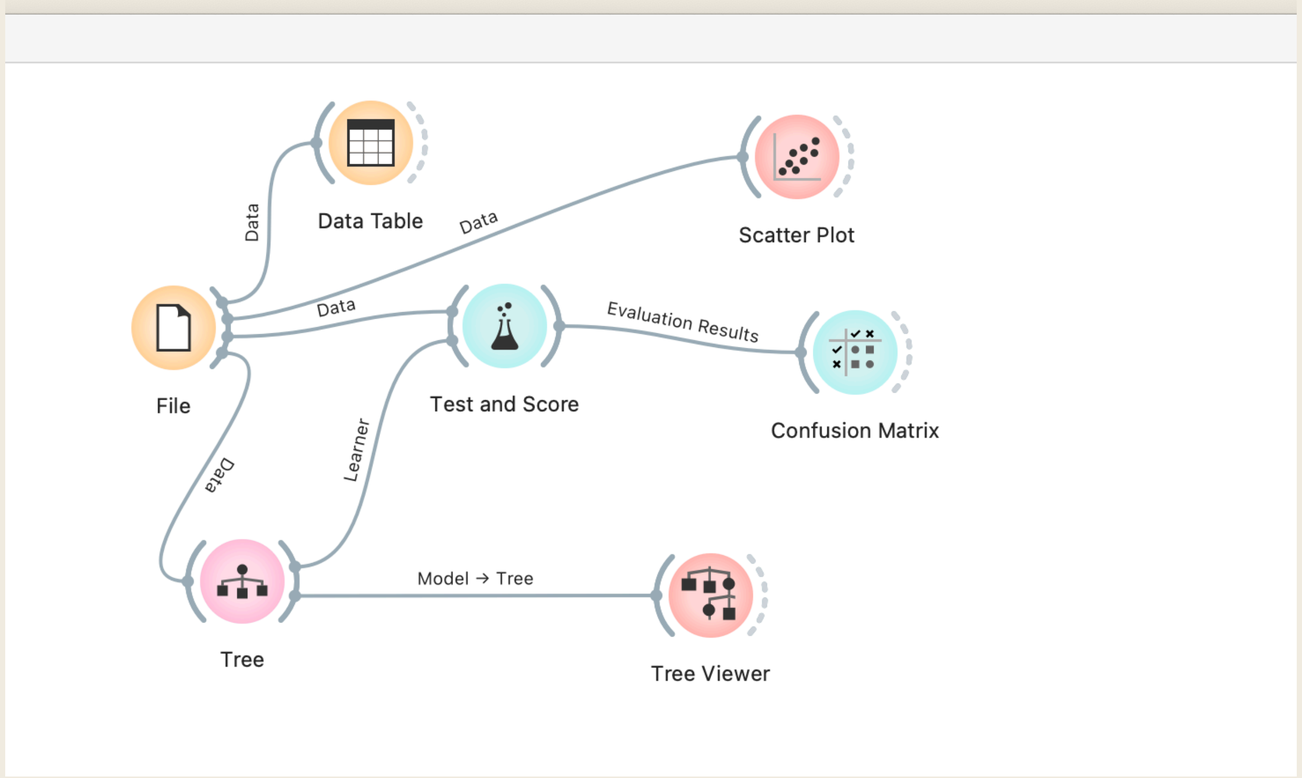
Gain (s, Sex)
= 0.940 – [(7/14)0.985 + (7/14)0.592]
=0.151

Gain (s, Cholesterol)
= 0.940 – [(8/14).811 + (6/14)1.0]
=0.048

The attribute more suitable give us the higher information gain . In this case "SEX"

Information gain is the information that can increase the level of certainty after splitting.

Information Gain = (Entropy before split) – (weighted entropy after split)



16/MARZO/2022

Decision Tree

- Datos de Iris
- Test and Score –> confusion Matrix
- Tree –> Tree Viewer

Linear Models
For classification

- Linear models are a class of models that are widely used in practice.
- Linear models make a prediction using a linear function of the input features

Linear Binary classification

In this case, the prediction is made using the formula:

$$\hat{y} = w[0] * x[0] + w[1]*x[1] + \ldots + w[p]*x[p] + b > 0$$

Where:

X [0,..p] are the features (columns)

W[0,..,p] and b are the parameters of the model

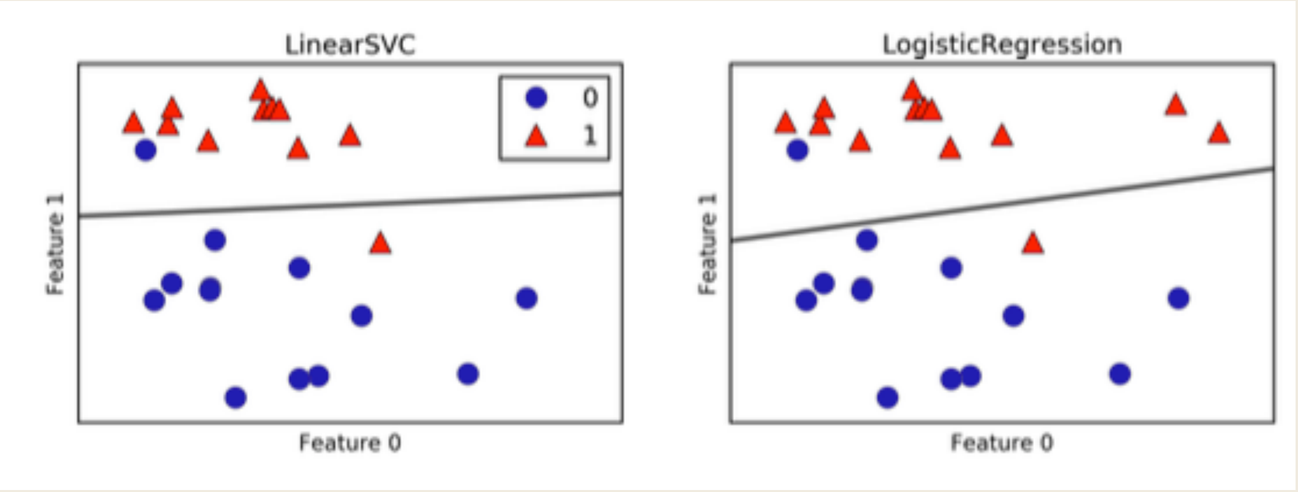
Y is the prediction of the model

Linear Models
For classification

A linear classifier is a classifier that separates two classes using a line, a plane or a hyperplane

The most common models:

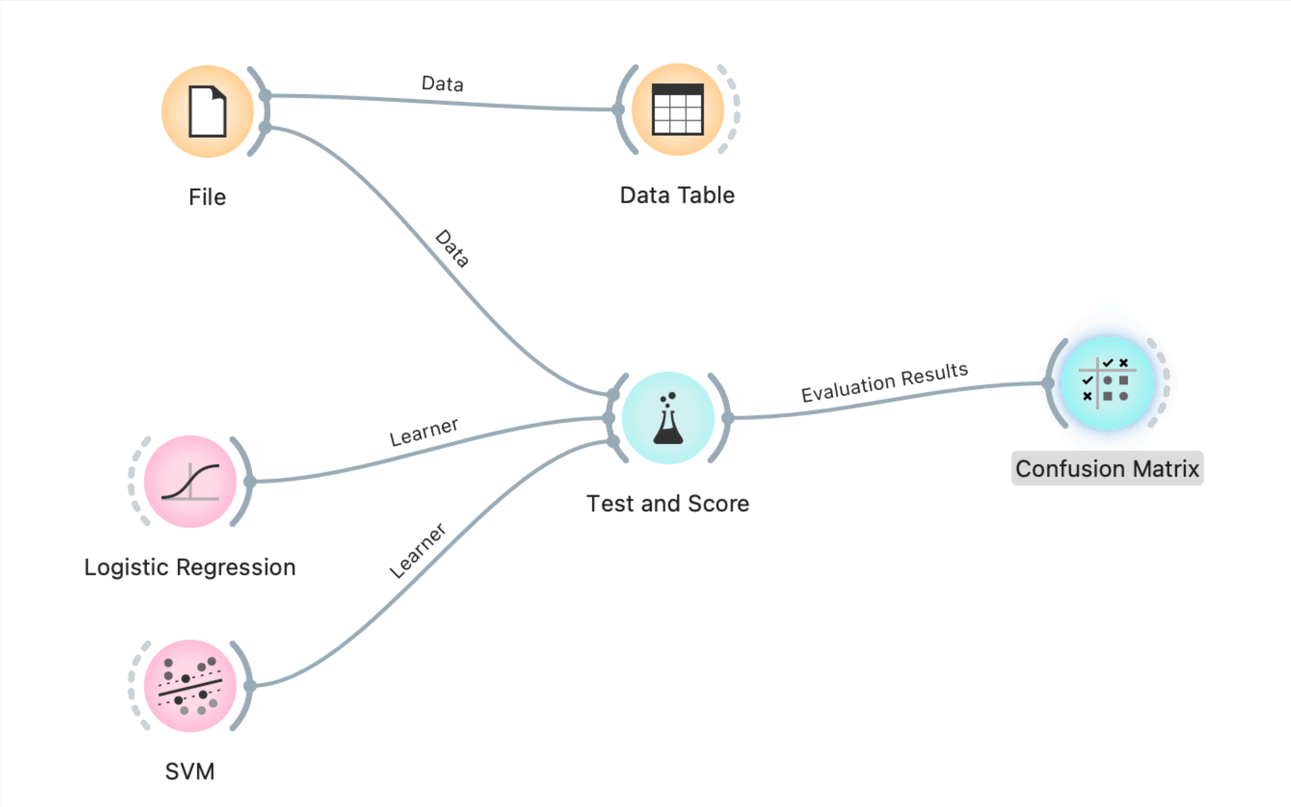
- Logistic Regression
- Support Vector Machine



16/MARZO/2022

Linear models

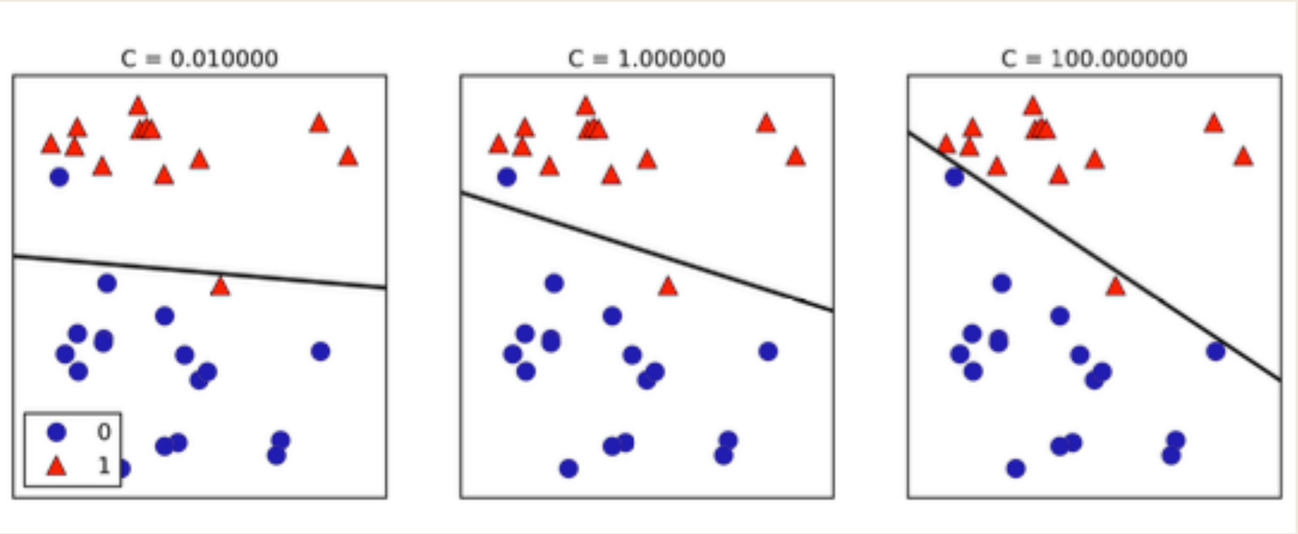
- Linear SVC
- Logistic Regression.



16/MARZO/2022

Linear Models

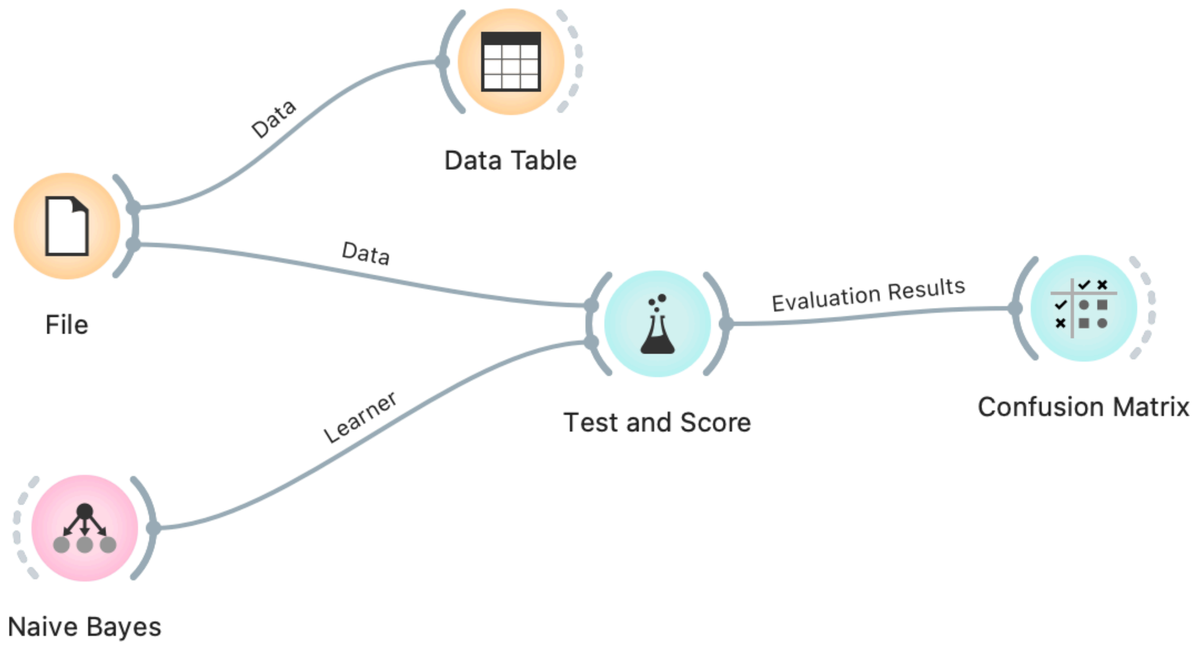
- Datos de Iris
- SVM -> Test and Score -> Confusion M.
- LR -> Test and Score -> Confusion M.
- C values
- Regularization type: L1, L2



16/MARZO/2022

Linear models

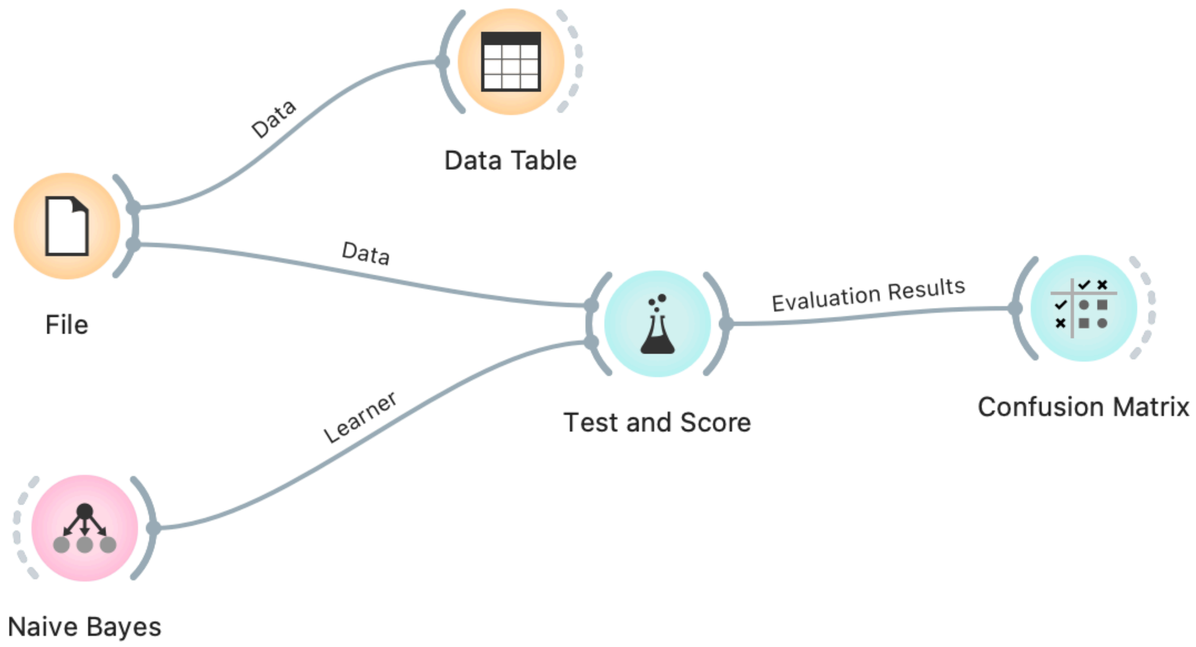
- Studying different C values
- Studying different regularizations.



16/MARZO/2022

Naive Bayes models

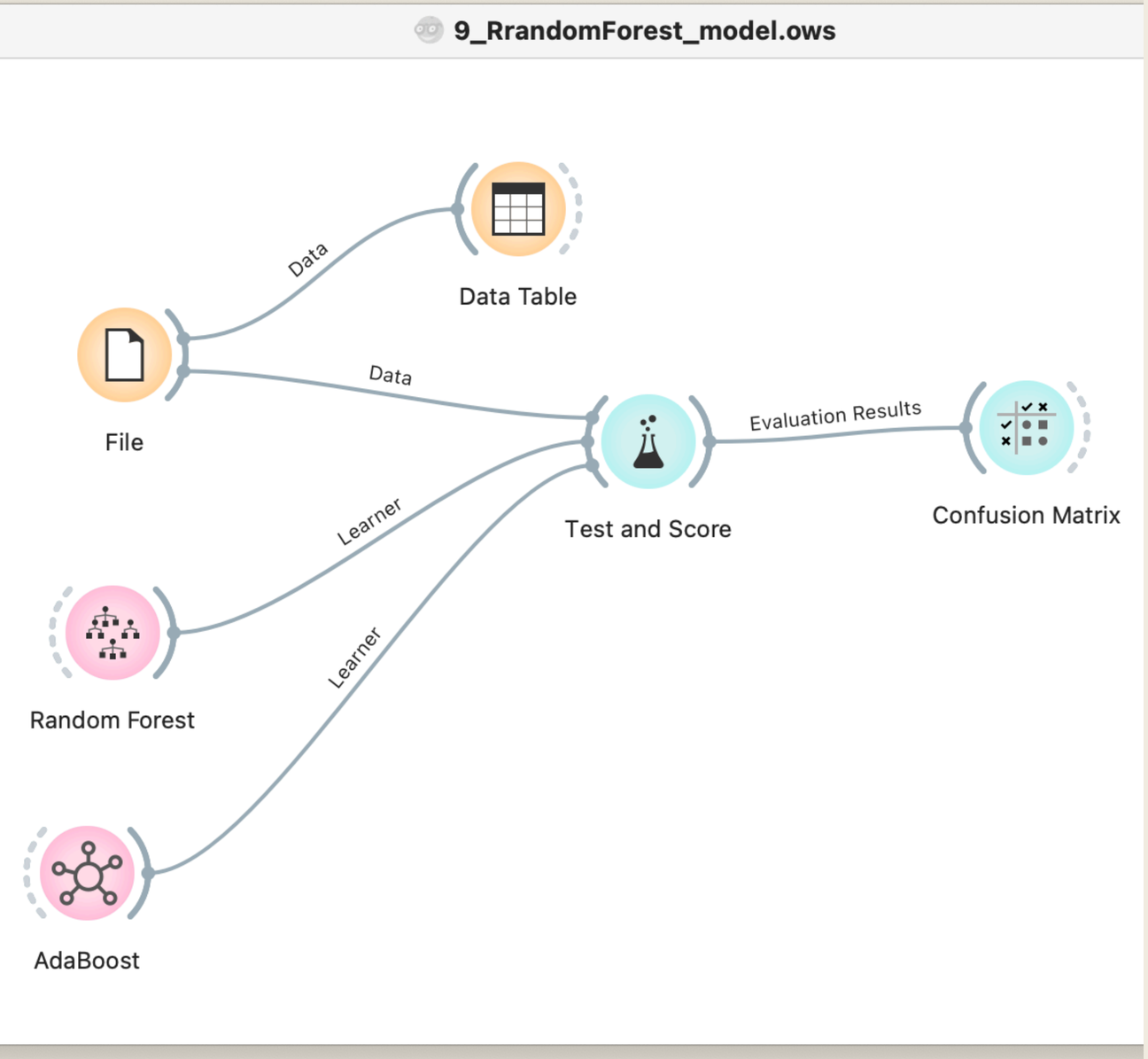
- Naive Bayes classifiers are a family of classifiers that are quite similar to the linear models.
- However, they tend to be even faster in training.
- The price paid for this efficiency is that naive Bayes models often provide generalization performance that is slightly worse than that of linear classifiers



16/MARZO/2022

Naive Bayes models

- There are three kinds of naive Bayes classifiers: **GaussianNB, BernoulliNB,** and **MultinomialNB**.
- GaussianNB can be applied to any continuous data, while BernoulliNB assumes binary data and MultinomialNB assumes count data
- Naive Bayes models are great baseline models and are often used on very large datasets, where training even a linear model might take too long.



16/MARZO/2022

Ensembles of Decision Trees

- Ensembles are methods that combine multiple machine learning models to create more powerful models.
- There are two ensemble models that have proven to be effective, both of which use decision trees as their building blocks: **random forests** and **gradient boosted decision trees.**

Random Forest

- The main drawback of decision trees is that they **tend to overfit** the training data. Random forests are one way to address this problem.
- A RF is essentially **a collection of decision trees**, where each tree is slightly different from the others. The idea behind random forests is that each tree might do a relatively good job of predicting, but will likely overfit on part of the data. If we build many trees, all of which work well and overfit in different ways, **we can reduce the amount of overfitting by averaging their results.**