

# Introduction to Machine Learning with Scikit-learn Part II: Simple classification models

For this second part of an introduction to the scikit-learn module, we will focus on the second type of problem in Machine Learning: the classification problem.

The objective of this introduction is to:

- Introduce the classification problem.
- Learn to use the scikit-learn module to build a classification model, also known as a "classifier"
- Introduce metrics adapted to the evaluation of classification models.

## Introduction to classification

#### Objective of classification

In supervised learning, the objective is to predict the value of a target variable from explanatory variables.

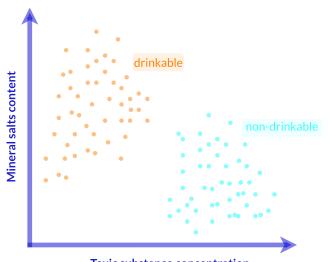
- In a **regression** problem, the target variable takes **continuous values**. These values are numerical: price of a house, quantity of oxygen in the air of a city, etc. The target variable can therefore take an **infinity of values**.
- In a classification problem, the target variable takes discrete values. These values
  can be numeric or literal, but in both cases the target variable takes a finite number
  of values.

The different values taken by the target variable are called classes.

The objective of classification therefore consists in predicting the class of an observation from its explanatory variables.

We will look at a problem of a **binary** classification, i.e. where there are **two** classes. We are trying to determine whether the water in a stream is drinkable or not depending on its concentration of toxic substances and its mineral salts content.

The two classes are therefore 'drinkable' and 'non-drinkable'.



Toxic substance concentration

In the figure above, each point represents a stream whose position on the map is defined by its values for the concentration of toxic substances and the content of mineral salts.

The objective will be to build a **model capable of assigning one of the two classes** ('drinkable' / 'non-drinkable') to a stream of which only these two variables are known.

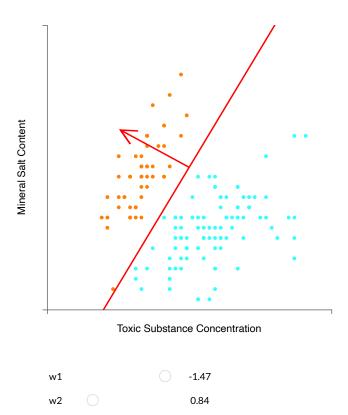
The figure above suggests the existence of two zones allowing easy classification of streams:

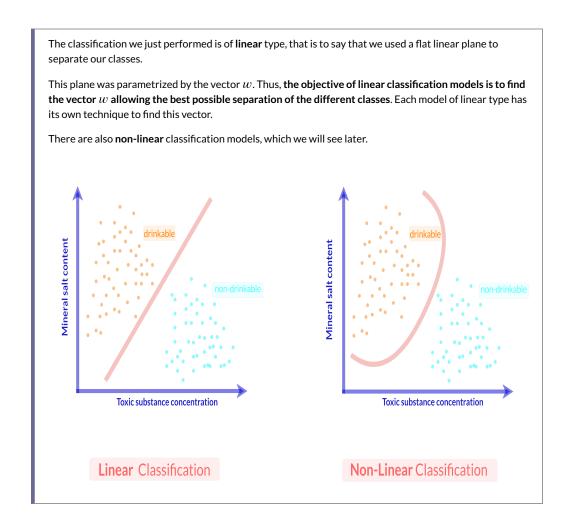
- An area where the streams are drinkable (top left).
- An area where the streams are not drinkable (bottom right).

We would like to create a model capable of **separating the dataset into two parts** corresponding to these areas.

A simple technique would be to separate the two areas using a line.

linear\_classification()





We will now introduce the main tools of the scikit-learn module for solving a classification problem.

In this exercise we will use the <u>Congressional Voting Records</u> (<a href="https://archive.ics.uci.edu/ml/datasets/congressional+voting+records">https://archive.ics.uci.edu/ml/datasets/congressional+voting+records</a>) dataset, containing a number of votes cast by members of Congress of the United States House of Representatives.

The objective of our classification problem will be to **predict the political party** ("Democrat" or "Republican") of the members of the House of Representatives according to their votes on subjects like the education, health, budget, etc.

The explanatory variables will therefore be the votes on various subjects and the target variable will be the "democrat" or "republican" political party.

To solve this problem we will use:

- A non-linear classification model: K-Nearest Neighbors.
- A linear classification model: Logistic Regression.

## **Data preparation**

• (a) Run the following cell to import the pandas and numpy modules needed for the exercise.

```
import pandas as pd
import numpy as np
```

%matplotlib inline

• (b) Load the data contained in the file 'votes.csv' into a DataFrame named votes.

```
In [8]:
```

```
# Insert your code here

votes = pd.read_csv('votes.csv')
votes
```

#### Out[8]:

	party	infants	water	budget	physician	salvador	religious	satellite	aid	missile	immigration	synfuels	education	su
0	republican	n	у	n	У	у	у	n	n	n	у	n	У	
1	republican	n	У	n	У	У	У	n	n	n	n	n	У	
2	democrat	n	У	У	n	у	у	n	n	n	n	у	n	
3	democrat	n	У	У	n	n	У	n	n	n	n	У	n	
4	democrat	У	У	У	n	У	У	n	n	n	n	У	n	
430	republican	n	n	У	У	У	У	n	n	У	У	n	У	
431	democrat	n	n	У	n	n	n	У	У	У	у	n	n	
432	republican	n	n	n	У	У	У	n	n	n	n	У	У	
433	republican	n	n	n	У	у	у	n	n	n	n	n	У	
434	republican	n	У	n	У	У	У	n	n	n	у	n	У	
435 r	435 rows × 17 columns													

Show solution

In order to briefly visualize our data:

• (c) Display the number of rows and columns of votes.

```
In [5]:
# Insert your code here
print(votes.shape)
#votes.head(20)
votes.head()
```

(435, 17)

#### Out[5]:

	party	infants	water	budget	physician	salvador	religious	satellite	aid	missile	immigration	synfuels	education	supe
0	republican	n	У	n	У	У	У	n	n	n	У	n	У	
1	republican	n	У	n	У	У	У	n	n	n	n	n	У	
2	democrat	n	У	У	n	У	У	n	n	n	n	У	n	
3	democrat	n	У	У	n	n	У	n	n	n	n	У	n	
4	democrat	У	У	У	n	У	У	n	n	n	n	У	n	

Hide solution

```
In [6]:
# Shape of the DataFrame
print('The DataFrame has', votes.shape[0], 'rows and', votes.shape[1], 'columns.')
# Display the first 20 rows
votes.head(20)
```

The DataFrame has 435 rows and 17 columns.

#### Out[6]:

	party	infants	water	budget	physician	salvador	religious	satellite	aid	missile	immigration	synfuels	education	sup
0	republican	n	У	n	У	У	у	n	n	n	У	n	У	
1	republican	n	У	n	У	У	у	n	n	n	n	n	У	
2	democrat	n	У	у	n	у	у	n	n	n	n	у	n	
3	democrat	n	У	У	n	n	у	n	n	n	n	у	n	
4	democrat	у	У	у	n	у	у	n	n	n	n	у	n	
5	democrat	n	У	У	n	у	у	n	n	n	n	n	n	
6	democrat	n	У	n	У	у	у	n	n	n	n	n	n	
7	republican	n	У	n	У	у	у	n	n	n	n	n	n	
8	republican	n	У	n	У	у	у	n	n	n	n	n	У	
9	democrat	У	У	У	n	n	n	у	У	У	n	n	n	
10	republican	n	У	n	У	у	n	n	n	n	n	n	n	
11	republican	n	У	n	У	у	у	n	n	n	n	у	n	
12	democrat	n	У	У	n	n	n	у	У	У	n	n	n	
13	democrat	У	У	У	n	n	У	у	У	n	У	у	n	
14	republican	n	У	n	У	у	у	n	n	n	n	n	У	
15	republican	n	У	n	У	У	У	n	n	n	У	n	У	
16	democrat	У	n	У	n	n	у	n	У	n	У	у	У	
17	democrat	у	n	У	n	n	n	у	У	у	n	n	n	
18	republican	n	У	n	у	у	у	n	n	n	n	n	n	
19	democrat	У	У	У	n	n	n	У	У	У	n	У	n	

Congress of the House of Representatives belongs. This is the target variable.

- The following 16 columns contain the votes of each member of Congress on legislative proposals:
  - 'y' indicates that the elected member voted for the bill.
  - 'n' indicates that the elected member voted against the bill.

In order to use the data in a classification model, it is necessary to transform these columns into binary **numeric** values, i.e. either 0 or 1.

- (e) For each of the columns 1 to 16 (column 0 being our target variable), replace the values 'y' by 1 and 'n' by 0. To do so, we can use the **replace** method from the <code>DataFrame</code> class.
- (f) Display the first  $10 \text{ rows of the modified } \mathtt{DataFrame}$  .

```
In [93]:
    # Insert your code here
    lst = ['y', 'n']
    df = votes.copy()

    df = df.iloc[: ,1:].replace('y', 1).replace('n', 0)
    # df.replace(('y', 'n'), (1,0)) # better
    df.head(10)
```

#### Out[93]:

•	infants	water	budget	physician	salvador	religious	satellite	aid	missile	immigration	synfuels	education	superfund	crim
0	0	1	0	1	1	1	0	0	0	1	0	1	1	
1	0	1	0	1	1	1	0	0	0	0	0	1	1	
2	0	1	1	0	1	1	0	0	0	0	1	0	1	
3	0	1	1	0	0	1	0	0	0	0	1	0	1	(
4	1	1	1	0	1	1	0	0	0	0	1	0	1	
5	0	1	1	0	1	1	0	0	0	0	0	0	1	
6	0	1	0	1	1	1	0	0	0	0	0	0	0	
7	0	1	0	1	1	1	0	0	0	0	0	0	1	
8	0	1	0	1	1	1	0	0	0	0	0	1	1	
9	1	1	1	0	0	0	1	1	1	0	0	0	0	t

Hide solution

```
votes = votes.replace(('y', 'n'), (1, 0))
# Display the first 10 rows of the DataFrame
votes.head(10)
```

#### Out[94]:

	party	infants	water	budget	physician	salvador	religious	satellite	aid	missile	immigration	synfuels	education	supe
0	republican	0	1	0	1	1	1	0	0	0	1	0	1	
1	republican	0	1	0	1	1	1	0	0	0	0	0	1	
2	democrat	0	1	1	0	1	1	0	0	0	0	1	0	
3	democrat	0	1	1	0	0	1	0	0	0	0	1	0	
4	democrat	1	1	1	0	1	1	0	0	0	0	1	0	
5	democrat	0	1	1	0	1	1	0	0	0	0	0	0	
6	democrat	0	1	0	1	1	1	0	0	0	0	0	0	
7	republican	0	1	0	1	1	1	0	0	0	0	0	0	
8	republican	0	1	0	1	1	1	0	0	0	0	0	1	
9	democrat	1	1	1	0	0	0	1	1	1	0	0	0	

- **(g)** In a DataFrame named X , store the **explanatory** variables of the dataset (all columns except 'party'). For this, you can use the **drop** method of a DataFrame.
- (h) In a DataFrame named y, store the target variable ('party').

```
In [102]:
# Insert your code here

X = votes.drop(['party'], axis=1)

y = votes['party']
```

Hide solution

```
In [103]:
# Separation of the variables

X = votes.drop(['party'], axis = 1)
y = votes['party']
```

As for the regression problem, we will have to split the data set into 2 sets: a **training set** and a **test set**. As a reminder:

- The training set is used to train the classification model, that is to say find the
  parameters of the model which best separate the classes.
- The test set is used to evaluate the model on data that it has never seen. This
  evaluation will allow us to judge the generalizability of the model.
- (i) Import the train\_test\_split function from the sklearn.model\_selection submodule. Remember that this function is used as follows:

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_siz
e = 0.2)
```

• (j) Split the data into a training set (X\_train, y\_train) and a test set (X\_test, y\_test) keeping 20% of the data for the test set.

use the function with the argument random\_state = 2, the datasets produced will be the same.

#### In [104]:

```
# Insert your code here
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2)
```

Hide solution

#### In [105]:

```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state =
```

#### Non-linear classification: K-Nearest Neighbors model

In order to assign a class to an observation, the K-Nearest Neighbors algorithm considers, as its name suggests, the **K nearest neighbors** of the observation and determines **the most represented class** among these neighbors.

Concretely, the algorithm is as follows:

- Suppose that K = 5.
- For an observation that we want to classify, we will look at the 5 points of the training set that are closest to our observation. The distance metric used is often the euclidian norm.
- If among the 5 neighbors, the majority is "democrat", then the observation will be classified "democrat".

To train a K-Nearest Neighbors model for our problem, we'll use the  ${\tt KNeighborsClassifer}$  class from the neighbors submodule of  ${\tt scikit-learn}$ .

The number K of neighbors to consider is entered using the parameter  $n\_neighbors$  of the KNeighborsClassifer constructor.

- (k) Run the following cell to import the  ${\tt KNeighborsClassifer}$  class.

#### In [106]:

from sklearn.neighbors import KNeighborsClassifier

- (I) Instantiate a KNeighborsClassifier model named knn which will consider the 6 nearest neighbors for classification.
- (m) Using the fit method, train the model knn on the training dataset.
- (n) Using the predict method, perform a prediction on the test dataset. Store these predictions in y\_pred\_test\_knn and display the first 10 predictions.

```
knn = KNeighborsClassifier(n_neighbors = 6)
knn.fit(X_train, y_train)
y_pred_test_knn = knn.predict(X_test)
y_pred_test_knn[:10]
```

Hide solution

In [111]:

```
# Instanciation du modèle
knn = KNeighborsClassifier(n_neighbors = 6)

# Entraînement du modèle sur le jeu d'entraînement
knn.fit(X_train, y_train)

# Prédiction sur les données de test
y_pred_test_knn = knn.predict(X_test)

# Affichage des 5 premières prédictions
print(y_pred_test_knn[:10])
```

```
['democrat' 'democrat' 'democrat' 'democrat' 'democrat'
'democrat' 'democrat' 'republican' 'democrat']
```

In the last part of this exercise, we will see how to evaluate the performance of our model using these predictions.

The logistic regression model is closely related to the **linear regression** model seen in the previous notebook.

They should not be confused since they do not solve the same types of problems:

- Logistic Regression is used for classification (predict classes).
- Linear regression is used for regression (predict a quantitative variable).

```
['democrat' 'republican' 'democrat' 'democrat' 'democrat' 'democrat' 'democrat' 'democrat']
```

# Entraînement du modèle sur le jeu d'entraînement

logreg.fit(X\_train, y\_train)

print(y pred test logreg[:10])

# Prédiction sur les données de test
y\_pred\_test\_logreg = logreg.predict(X\_test)

# Affichage des 5 premières prédictions

There are different metrics to evaluate the performance of classification models such as:

- The accuracy.
- The precision and the recall.
- The F1-score.

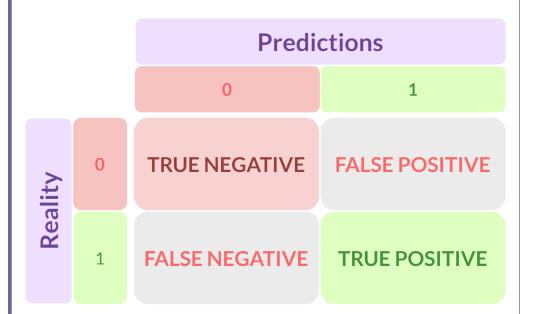
Each metric assesses the performance of the model with a different approach.

In order to explain these concepts, we will introduce 4 very important terms.

Arbitrarily, we will choose that the class 'republican' will be the positive class (1) and 'democrat' will be the negative class (0).

Thus, we will call:

- True Positive (TP) an observation classified as positive ('republican') by the model which is indeed positive ('republican').
- False Positive (FP) an observation classified as positive ('republican') by the model which was actually negative ('democrat').
- True Negative (TN) an observation classified as negative ('democrat') by the model and which is indeed negative ('democrat').
- False Negative (FN) an observation classified as negative ('democrat') by the model which was actually positive ('republican').



The accuracy is the most common metric used to evaluate a model. It simply corresponds to the rate of correct predictions made by the model.

We suppose that we have n observations. We denote by TP the number of True Positives and TN the number of True Negatives. Then the accuracy is given by:

$$accuracy = \frac{TP + TN}{n}$$

The precision is a metric which answers the question: Among all the positive predictions of the model, how many are true positives? If we denote by FP the number of False Positives of the model, then the precision is given by:

$$precision = \frac{TP}{TP + FP}$$

A high precision score tells us the model does not blindly classify everyone as positive.

If we write FN as the number of False Negatives, then the callback is given by:

$$recall = \frac{TP}{TP + FN}$$

A high recall score tells us the model is able to properly detect the truly positive observations.

The confusion matrix counts the values of TP, TN, FP and FN for a set of predictions, which allows us to calculate the three previous metrics:

$$ConfusionMatrix = \begin{bmatrix} TN & FP \\ FN & TP \end{bmatrix}$$

The confusion\_matrix function of the sklearn.metrics submodule generates the confusion matrix from the **predictions** of a model:

```
confusion_matrix (y_true, y_pred)
```

As a reminder:

- y\_true contains the true values of y.
- y\_pred contains the values of y predicted by the model.
- (a) Import the confusion\_matrix function from sklearn.metrics.
- (b) Calculate the confusion matrix of the predictions produced by the model knn . These predictions were stored in y\_pred\_test\_knn.
- (c) Display the confusion matrix. How many false positives have occurred? The positive class corresponds to 'republican'.
- (d) Using the formulas given above, calculate the accuracy, precision, and recall scores of the knn model on the test set. You can use tuple assignment to deconstruct the confusion matrix:

```
(TN, FP), (FN, TP) = confusion_matrix(y_true, y_pred)
```

```
In [136]:
```

```
# Insert your code here
 # NOTE
 # 'republican' = 1
 # 'democrat' = 0
 from sklearn.metrics import confusion_matrix
 y_pred_test_knn = knn.predict(X_test)
 cm = confusion_matrix(y_test, y_pred_test_knn)
 print('confusion_matrix : \n', cm)
 print(cm[0])
 print(cm[0,0])
 (TN, FP), (FN, TP) = confusion_matrix(y_test, y_pred_test_knn)
 accuracy = (TP + TN) / len(y_test)
 precision = TP / (TP + FP)
 recall = TP / (TP + FN)
 print('Accuracy :', accuracy, '\nPrecision :', precision, '\nRecall :', recall)
confusion_matrix :
[[48 5]
[ 3 31]]
```

https://train.datascientest.com/hub/abdullahcay26@gmail.com/notebooks/179/124#

Accuracy: 0.9080459770114943 Precision: 0.8611111111111112 Recall: 0.9117647058823529

[48 5] 48

In [135]:

```
from sklearn.metrics import confusion_matrix

# Computation and display of the confusion matrix
conf_matrix = confusion_matrix(y_test, y_pred_test_knn)
print("Confusion Matrix:\n", conf_matrix)

print("\nThe knn model made", conf_matrix[0,1], "False Positives.")

# Computation of the accuracy, precision and recall
(TN, FP), (FN, TP) = confusion_matrix(y_test, y_pred_test_knn)
n = len(y_test)

print("\nKNN Accuracy:", (TP + TN) / n)

print("\nKNN Precision:", TP / (TP + FP))

print("\nKNN Recall:", TP / (TP + FN))
```

```
Confusion Matrix:
[[48 5]
[ 3 31]]

The knn model made 5 False Positives.

KNN Accuracy: 0.9080459770114943

KNN Precision: 0.861111111111112

KNN Recall: 0.9117647058823529
```

The display of the confusion matrix can also be done with the **pd.crosstab** function as we had done in a previous notebook:

```
pd.crosstab(y_test, y_pred_test_knn, rownames = ['Reality'], colnames
= ['Prediction'])
```

Which in our case will produce the following DataFrame:

Prediction democrat republican

Reality		
democrat	48	5
republican	2	32

For this dataset, the KNN model performs quite well. When the classes are **balanced**, i.e. there are about as many positives as there are negatives in the dataset, accuracy is a good enough metric to assess the performance.

However, as you will see later, when a class is dominant, precision and recall are much more relevant metrics.

If you think you cannot remember the formulas for the metrics of accuracy, precision and recall, do not worry! The **sklearn.metrics** submodule contains functions to calculate them quickly:

```
accuracy_score(y_test, y_pred_test_knn) >>> 0.9195402298850575
```

- (e) Import the accuracy\_score, precision\_score and recall\_score functions from the sklearn.metrics submodule.
- (f) Display the confusion matrix of the predictions made by the logreg model using pd.crosstab.
- (g) Calculate the accuracy, precision and recall of model predictions logreg. To use the precision\_score and recall\_score metrics, you will need to fill in the argument pos\_label = 'republican' in order to specify that the 'republican' class is the positive class.

```
from sklearn.metrics import accuracy_score, precision_score, recall_score
knn_crosstab = pd.crosstab(y_test, y_pred_test_knn, rownames = ['Reality'], colnames = ['print(knn_crosstab)

accuracy_score = accuracy_score(y_test, y_pred_test_knn)
precision_score = precision_score(y_test, y_pred_test_knn, pos_label = 'republican')
recall_score = recall_score(y_test, y_pred_test_knn, pos_label = 'republican')
print('Accuracy Score : ', accuracy_score, '\nPrecison Score : ', precision_score, '\nRec
```

Prediction democrat republican
Reality
democrat 48 5
republican 3 31
Accuracy Score: 0.9080459770114943
Precison Score: 0.86111111111111112
Recall Score: 0.9117647058823529

Hide solution

#### In [142]:

```
from sklearn.metrics import accuracy_score, precision_score, recall_score

# Computation and display of the confusion matrix
pd.crosstab(y_test, y_pred_test_logreg, rownames=['Reality'], colnames=['Prediction'])

# Computation of the accuracy, precision and recall
print("\nLogReg Accuracy:", accuracy_score(y_test, y_pred_test_logreg))

print("\nLogReg Precision:", precision_score(y_test, y_pred_test_logreg, pos_label = 'rep
print("\nLogReg Recall:", recall_score(y_test, y_pred_test_logreg, pos_label = 'republica')
```

The **classification\_report** function of the sklearn.metrics submodule displays all these metrics for each class.

- (h) Import the classification\_report function from the sklearn.metrics submodule.
- (i) Display using the print and classification\_report functions the classification reports of the models logreg and knn on the test set.

```
from sklearn.metrics import classification_report
print('Logistic Regresion Report: \n', classification_report(y_test, y_pred_test_logreg))
print('\nKNN Report: \n', classification_report(y_test, y_pred_test_knn))
```

Logistic Regre	esion Report:			
	precision	recall	f1-score	support
democrat	0.96	0.92	0.94	53
republican	0.89	0.94	0.91	34
accuracy			0.93	87
macro avg	0.92	0.93	0.93	87
weighted avg	0.93	0.93	0.93	87
KNN Report:				
	precision	recall	fl-score	support
democrat	0.94	0.91	0.92	53
republican	0.86	0.91	0.89	34
accuracy			0.91	87
macro avg	0.90	0.91	0.90	87
weighted avg	0.91	0.91	0.91	87

Hide solution

```
In [165]:
```

```
from sklearn.metrics import classification_report
print("LogReg report:\n", classification_report(y_test, y_pred_test_logreg))
print("\n\n")
print("KNN report:\n", classification_report(y_test, y_pred_test_knn))
```

#### LogReg report:

	precision	recall	f1-score	support
democrat	0.96	0.92	0.94	53
republican	0.89	0.94	0.91	34
accuracy			0.93	87
macro avg	0.92	0.93	0.93	87
weighted avg	0.93	0.93	0.93	87

#### KNN report:

	precision	recall	f1-score	support
democrat	0.94	0.91	0.92	53
republican	0.86	0.91	0.89	34
accuracy			0.91	87
macro avg	0.90	0.91	0.90	87
weighted avg	0.91	0.91	0.91	87

The classification report is a little more complete than what we have done so far. It contains an additional metric: the **F1-Score**.

The F1-Score is a sort of average between precision and recall. The F1-Score adapts very well to classification problems with balanced or unbalanced classes.

For most classification problems, the model with the highest F1-Score will be considered the model whose recall and precision **performances** are the most **balanced**, and is therefore **preferable** to others.

As for the recall and the precision, it will be necessary to fill in the argument  $pos\_label = "republican"$ .

```
In [175]:
# Insert your code here
from sklearn.metrics import f1_score
print('Log. Reg. F1_score : ', f1_score(y_test, y_pred_test_logreg, pos_label = 'republic
print('KNN F1_score : ', f1_score(y_test, y_pred_test_knn, pos_label = 'republican'

Log. Reg. F1_score : 0.9142857142857143
KNN F1_score : 0.8857142857142858

Hide solution

In [176]:
from sklearn.metrics import f1_score
print("F1 KNN:", f1_score(y_test, y_pred_test_knn, pos_label = 'republican'))
print("F1 LogReg:", f1_score(y_test, y_pred_test_logreg, pos_label = 'republican'))

F1 KNN: 0.8857142857142858
F1 LogReg: 0.9142857143
```

# **Conclusion and recap**

- $\bullet \quad \mathsf{Linear}\, \mathbf{models}\, \mathsf{like}\,\, \mathbf{LogisticRegression}\,\,.$
- Non-linear models like KNeighborsClassifier.

The implementation of these models is done in the same way for all models of scikit-learn:



Validate