





Dados e Aprendizagem Automática Quality Metrics and Model Validation

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- A Machine Learning Algorithm (Decision Trees)
- Quality Metrics
- Model Validation
- Hands On

A Machine Learning Algorithm

Today we will be "playing" with Decision Trees!

You don't know what that means? Don't worry, we will see it soon! For now, you just need to know that it is a model that predicts the value of a target feature:

• A Decision Tree is a hierarchical graph (it's a tree)!

Each branch represents a selection among a set of alternatives;

Each leaf node represents a class.



A Machine Learning Algorithm - Classifier

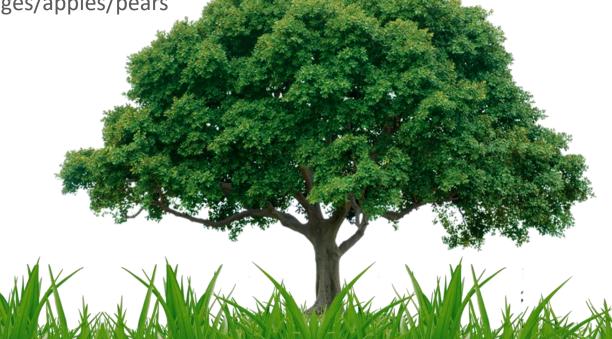
We can have a Decision Tree classifier, which is used for classification problems (the target feature is a class):

• Deciding if we should have lunch - binary classification - Yes/No

Surviving the Titanic - again, binary classification - 1/0

Classify a set of images - multiclass classification - oranges/apples/pears

•



A Machine Learning Algorithm - Regressor

But we can also have a Decision Tree regressor, which is used for regression problems (the target feature is real/continuous):

- Predict the traffic flow (km/h)
- Predict stock prices (€)
- •



Implementing a Decision Tree Classifier - Data Loading

Let's use the Titanic dataset and start by loading the dataset:

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We now need to define our input and our target features!

X is typically used to identify the input. y to identify the target.

```
#Let's start by creating our X (input data) and our y (target feature - the Survived feature)
X = df.drop(['Survived'], axis=1)  #input features - everything except the Survived feature
y = df['Survived'].to_frame()  #target feature
```

X

	Passengerld	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
0	1	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	NaN	S
1	2	1	Cumings, Mrs. John Bradley (Florence Briggs Th	female	38.0	1	0	PC 17599	71.2833	C85	С
2	3	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	NaN	S
3	4	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S
4	5	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S
	. 8	91 rows	× 11 columns			•••	•••			•••	

We now need to define our input and our target features!

X is typically used to identify the input. y to identify the target.

```
#Let's start by creating our X (input data) and our y (target feature - the Survived feature)
X = df.drop(['Survived'], axis=1)  #input features - everything except the Survived feature
y = df['Survived'].to_frame()  #target feature
```

у

Survived

0	0
1	1
2	1
3	1
4	0

··· 891 rows × 1 columns

Implementing a Decision Tree Classifier - Train/Test split

Both the X and the y have 891 rows of data - that corresponds to the entire dataset!

Hence, our next step is to leave aside a small set of data to test/validate the model (25%), like this:

```
#Let's use the X and Y, which contain 891 rows of data
#to create train and test sets of data.
#Important -> Define the random_state for reproducibility
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.25, random_state=2021)

print("The shape of X %s. X_train has shape %s while X_test has shape %s" %(X.shape, X_train.shape, X_test.shape))
The shape of X (891, 11). X_train has shape (668, 11) while X_test has shape (223, 11)

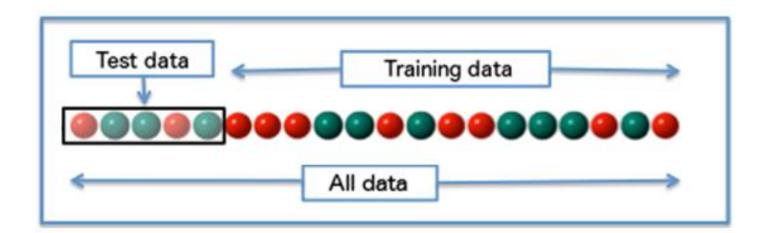
print("The shape of y %s. y_train has shape %s while y_test has shape %s" %(y.shape, y_train.shape, y_test.shape))
The shape of y (891, 1). y_train has shape (668, 1) while y_test has shape (223, 1)
```

Amount of data for testing 25%

Random seed

Hold-out Validation

In essence, what we have done means we will validate the model on unseen data, i.e., we use a "partitioning method" to split the training and the testing data once. This means we hold-out a subset of data for testing (80/20; 75/25; 65;35...).



Implementing a Decision Tree Classifier - Model Fitting

How can we now use a DT to predict whether a passenger would survive the disaster?

We first create an instance of the classifier and then we use the fit function.

```
#Create an instance of a Decision Tree classifier

#Again, defining the random_state for reproducibility

clf = DecisionTreeClassifier(random_state=2021)
```

```
#Training, i.e., fitting the model (using the training data!!)
clf.fit(X_train, y_train)
```

Implementing a Decision Tree Classifier - Model Fitting

```
Ups!!
#Create an instance of a Decision Tree classifier
#Again, defining the random state for reproducibility
clf = DecisionTreeClassifier(random state=2021)
#Training, i.e., fitting the model (using the training data!!)
clf.fit(X train, y train)
                                          Traceback (most recent call last)
ValueError
~\AppData\Local\Temp/ipykernel 1796/2168925757.py in <module>
      1 #Training, i.e., fitting the model (using the training data!!)
----> 2 clf.fit(X train, y train)
ValueError: could not convert string to float: 'Ali, Mr. William'
```

Sklearn decision trees do not handle categorical data (see issue #12866)!! (https://github.com/scikit-learn/scikit-learn/pull/12866)

Implementing a Decision Tree Classifier - Model Fitting

We could use techniques such as Label or One-Hot encoding to handle categorical data! For now, let's just drop those features.

```
X_train = X_train.drop(['Name', 'Sex', 'Age', 'Ticket', 'Cabin', 'Embarked'], axis=1)
X_test = X_test.drop(['Name', 'Sex', 'Age', 'Ticket', 'Cabin', 'Embarked'], axis=1)
#Training, i.e., fitting the model (using the training data!!)
```

DecisionTreeClassifier(random state=2021)

clf.fit(X train, y train)

#dropping categorical features from the input data (X train and X test)

Implementing a Decision Tree Classifier - Prediction

1, 1, 1, 1, 0, 0, 0, 1, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0,

1, 1, 0], dtype=int64)

With the model fitted, we can use the **predict function** to obtain the prediction of survival for each row/observation in the test set (0 - doesn't survive; 1 - survives).

We now have predictions for the test set (and we know the actual survival value as it is stored in the y test variable). How do we evaluate our classification model? There are some options...

Quality Metrics and Model Evaluation

But first... Why quality metrics?

How else would we quantify the model's performance? Metrics are used to monitor and measure the performance of a model. Some metrics are the Mean Absolute Error, the Mean Squared Error, Accuracy, F1-Score, ... There are many!

However, it depends on the problem in hands. Is it a classification problem? A regression one? A time series?



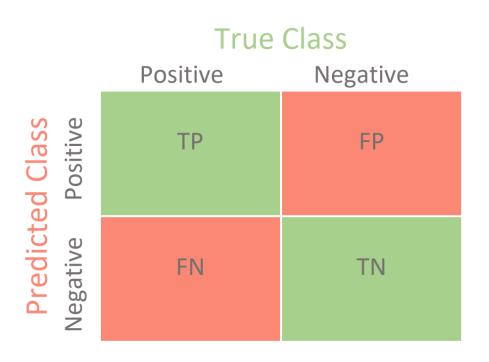
Quality Metrics

- Confusion Matrix
- Accuracy
- Precision
- Recall
- ROC
- AUC
- F₁ Score
- F_{β} Score

- MAE
- MSE
- RMSE

Classification Models - Confusion Matrix

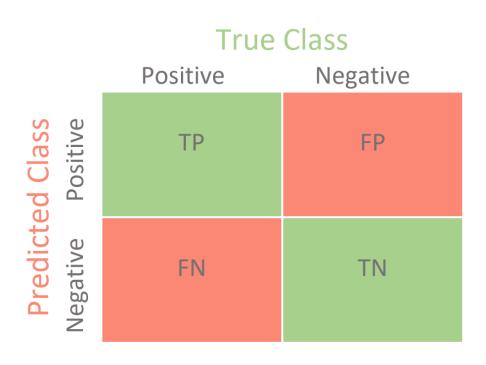
A confusion matrix is a table that is used to describe the performance of a classification model on a set of test data for which the true values are, again, known.



Accuracy

Accuracy is simply calculated as the number of all correct predictions divided by the total number of observations.

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$



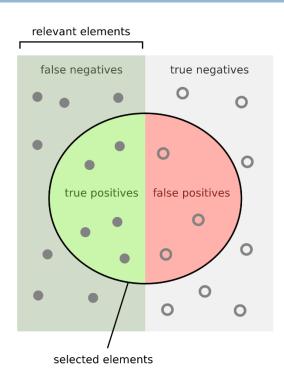
Precision and Recall

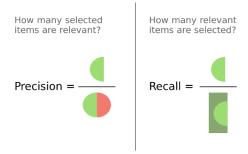
Precision (aka Sensitivity) is a measure of exactness, determines the fraction of relevant items among the retrieved items.

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

Recall (aka Specificity) is a measure of completeness, determines the fraction of relevant items that were obtained.

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





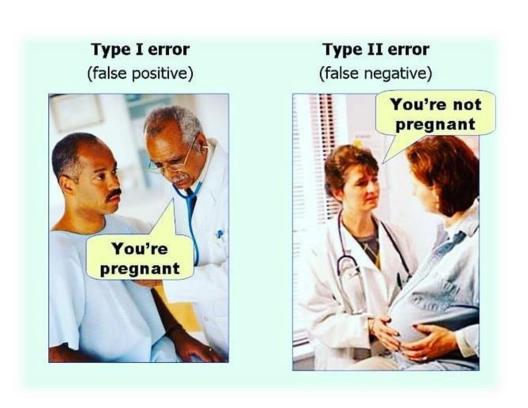
Precision and Recall

Precision (aka Sensitivity) is a measure of exactness, determines the fraction of relevant items among the retrieved items.

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

Recall (aka Specificity) is a measure of completeness, determines the fraction of relevant items that were obtained.

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



Confusion Matrix-based Metrics

Obtaining the confusion matrix is as simple as...

```
confusion_matrix(y_test, predictions)
array([[96, 39],
      [43, 45]], dtype=int64)
```

The same for the model's accuracy, precision, and recall!

```
0.6322869955156951

precision_score(y_test, predictions)
```

0.5357142857142857

accuracy score(y test, predictions)

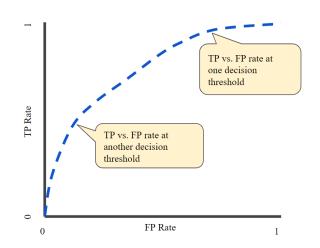
```
recall_score(y_test, predictions)
```

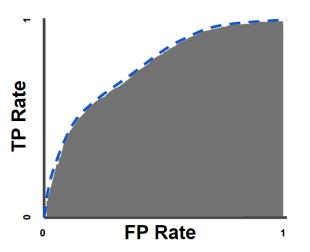
0.5113636363636364

ROC and AUC

The Receiver Operating Characteristics (ROC) curve finds the performance of a classification model at different classification thresholds. Lowering the classification threshold classifies more items as positive, thus increasing both False Positives and True Positives.

The Area Under the Curve (AUC) measures the two-dimensional area underneath the ROC curve (think integral calculus). It measures how well predictions are ranked, rather than their absolute values, and ranges from 0 to 1. A model whose predictions are 100% wrong has an AUC of 0; one whose predictions are 100% correct has an AUC of 1.





ROC and AUC

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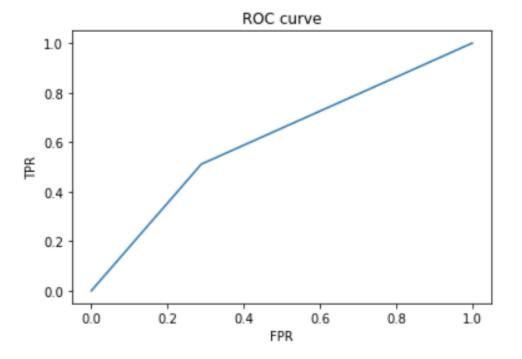
As for the ROC and the AUC...

```
roc_auc_score(y_test, predictions)
```

0.6112373737373737

```
fpr, tpr, _ = roc_curve(y_test, predictions)

plt.clf()
plt.plot(fpr, tpr)
plt.xlabel('FPR')
plt.ylabel('TPR')
plt.title('ROC curve')
plt.show()
```



F_1 and F_β Score

The F_1 Score combines precision and recall into a single value for comparison purposes. Can be used to obtain a more balanced view of performance.

$$F_1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall}$$

The F_1 Score gives equal weight to precision and recall. Use F_β Score to weight recall by a factor of β . With $\beta=1$, F_1 and F_β are equivalent.

$$F_{\beta} = (1 + \beta^{2}) \cdot \frac{Precision \cdot Recall}{\beta^{2} \cdot Precision + Recall}$$

F_1 and F_β Score

As for the F_1 and F_β Score ...

```
f1_score(y_test, predictions)
```

0.5232558139534884

```
fbeta_score(y_test, predictions, beta=0.5)
```

0.5306603773584905

A Decision Tree Regressor

But let's say that we wanted to predict the FARE paid by those that went to the Titanic (maybe not a very good problem, but it serves its purpose)!

For that, we would need a Decision Tree regressor!



Implementing a Decision Tree Regressor

We first need to re-define our input (X) and our target (y) features!

```
#Let's assume a REGRESSION problem! Let's predict the FARE paid by a person
#(maybe not a very good problem but it serves its purpose)!
#Let's start by creating our X (input data) and our y (target feature - the Survived feature)
X = df.drop(['Fare'], axis=1)  #input features - everything except the Survived feature
y = df['Fare'].to_frame()  #target feature
```

And to hold-out some data for testing (and again drop the categorical features)!

```
#Let's use the X and Y, which contain 891 rows of data
#to create train and test sets of data.
#Important -> Define the random_state for reproducibility
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.25, random_state=2021)
#dropping categorical features from the input data (X_train and X_test)
X_train = X_train.drop(['Name', 'Sex', 'Age', 'Ticket', 'Cabin', 'Embarked'], axis=1)
X_test = X_test.drop(['Name', 'Sex', 'Age', 'Ticket', 'Cabin', 'Embarked'], axis=1)
```

Implementing a Decision Tree Regressor

Now, just fit and predict the fare paid by the people at the test set.

We now have fare predictions for the test set (and we know the actual fare value as it is stored in the y test variable). How do we evaluate our regression model? There are, again, some options...

Mean Absolute Error

MAE

Mean Absolute Error measures the average magnitude of the errors in a set of predictions, without considering their direction.

$$MAE = \frac{1}{n} \sum_{j=1}^{n} |y_j - \hat{y}_j|$$

Where n is the number of observations, and y_j and \hat{y}_j are the actual observation and the predicted value, respectively.

Mean Squared Error

MSE

Mean Squared Error consists of the average of squared differences between the prediction and the actual observation, without considering their direction.

$$MSE = \frac{1}{n} \sum_{j=1}^{n} (y_j - \hat{y}_j)^2$$

Where n is the number of observations, and y_j and \hat{y}_j are the actual observation and the predicted value, respectively.

Root Mean Squared Error

RMSE

Root Mean Squared Error consists of the square root of the average of squared differences between the prediction and the actual observation, without considering their direction.

$$RMSE = \sqrt{\frac{1}{n} \sum_{j=1}^{n} (y_j - \hat{y}_j)^2}$$

Where n is the number of observations, and y_j and \hat{y}_j are the actual observation and the predicted value, respectively.

Regression Quality Metrics

$$MAE = \frac{1}{n} \sum_{j=1}^{n} |y_j - \hat{y}_j| \qquad MSE = \frac{1}{n} \sum_{j=1}^{n} (y_j - \hat{y}_j)^2 \qquad RMSE = \sqrt{\frac{1}{n} \sum_{j=1}^{n} (y_j - \hat{y}_j)^2}$$

Important notes:

- Three of the most common metrics used to measure accuracy for continuous variables
- All express average model prediction error (lower values are better)
- All range from 0 to ∞ and are indifferent to the direction of errors
- MAE and RMSE express the prediction error in units of the variable of interest
- MSE and RMSE, by squaring the error, gives a relatively high weight to large errors
- Hence, MSE and RMSE are more useful when large errors are particularly undesirable

Regression Quality Metrics

$$MAE = \frac{1}{n} \sum_{j=1}^{n} |y_j - \hat{y}_j| \qquad MSE = \frac{1}{n} \sum_{j=1}^{n} (y_j - \hat{y}_j)^2 \qquad RMSE = \sqrt{\frac{1}{n} \sum_{j=1}^{n} (y_j - \hat{y}_j)^2}$$

#	Error	Error	Error ²
1	1	1	1
2	-1	1	1
3	3	3	9
4	3	3	9

#	Error	Error	Error ²		
1	0	0	0		
2	0	0	0		
3	0	0	0		
4	10	10	100		

MAE		MSE	RMSE		
	2	5	2.24		

Regression Quality Metrics

Obtaining the model's MSE, MAE, and RMSE is as simple as:

```
mean_absolute_error(y_test, predictions)
```

14.68592556053812

```
#squared parameter as TRUE for MSE
mean_squared_error(y_test, predictions, squared=True)
```

1399,7722041242152

```
#squared parameter as FALSE for RMSE
mean_squared_error(y_test, predictions, squared=False)
```

37.41352969347072

For example, the RMSE tells us that our mean error is of 37.41£ ...

Quality Metrics

Here are some basic functions/classes you'll need (somewhen) in the future:

- sklearn.metrics.accuracy_score
- sklearn.metrics.auc
- sklearn.metrics.mean_absolute_error
- sklearn.metrics.mean_squared_error
- sklearn.metrics.f1_score
- sklearn.metrics.make_scorer
- •

Imports

And here are (some of) the imports you may need:

```
from sklearn.model selection import train test split
from sklearn.tree import DecisionTreeClassifier
from sklearn.tree import DecisionTreeRegressor
from sklearn.metrics import confusion matrix
from sklearn.metrics import recall score
from sklearn.metrics import accuracy score
from sklearn.metrics import precision score
from sklearn.metrics import roc auc score
from sklearn.metrics import roc curve
from sklearn.metrics import f1_score
from sklearn.metrics import fbeta score
from sklearn.metrics import mean absolute error
from sklearn.metrics import mean_squared_error
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np
#USING CROSS VALIDATION
from sklearn.model selection import cross val score
```

What about model validation?

Well, we must confirm that the model actually achieves its intended purpose! The goal is to check the accuracy/performance of the model based on data the model doesn't know.

Until now, we have been using hold-out validation! But that's a very basic way to address the problem, right?

Do you see any problems with it?



- Hold-out Validation
- Cross Validation
- k-fold Cross Validation
- Leave-one-out Cross Validation
- •

Cross Validation

Cross validation is another model validation technique!

The goal is to have an accurate metric of how the model will perform in practice.

In essence, it consists in dividing the dataset into k folds. In each run of the model, k-1 folds are used for training and 1 fold (the remaining) is used as test. Keep repeating the process until all folds have been used for testing.

The final error metric is based on the mean value of all error metrics:

$$E = \frac{1}{k} \sum_{i=1}^{k} E_i$$

Cross Validation - How many folds?

Well, ...

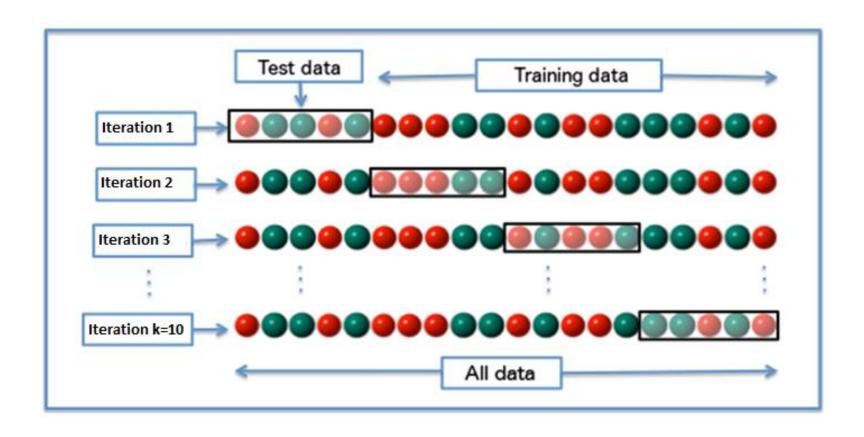
A greater number of folds will lead to a better error estimate of the model, a lower bias and less overfitting! However, it comes with a higher computational cost!

If we have a large dataset, a smaller k may be enough since we will have a larger amount of data for training. If we have a small dataset, we may want to use leave-one-out cross validation to maximize the amount of data for training...

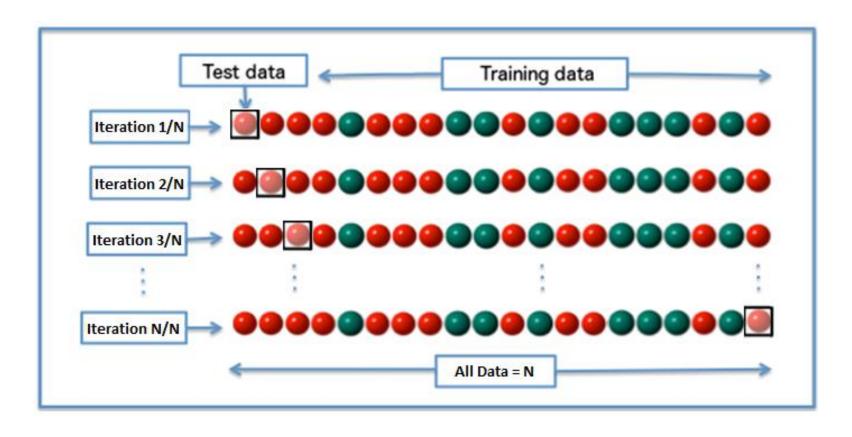
In reality, k depends on N!!
Rule of thumb -> k=10!

Row ID	D Error in %	Size of Test Set	Error Count
fold 0	38.281	128	49
fold 1	35.156	128	45
fold 2	44.531	128	57
fold 3	42.969	128	55
fold 4	42.969	128	55
fold 5	41.406	128	53
fold 6	41.406	128	53
fold 7	40.625	128	52
fold 8	41.406	128	53
fold 9	42.52	127	54

k-fold Cross Validation



Leave-one-out Cross Validation (k=N)



The special case of having k=N. Expensive...

But a good approach when we have a small dataset.

Here are some basic functions/classes you'll need (somewhen) in the future:

- sklearn.model_selection.train_test_split
- sklearn.model_selection.Kfold
- sklearn.model_selection.LeaveOneOut
- sklearn.model_selection.StratifiedKFold
- sklearn.model_selection.GridSearchCV
- sklearn.model_selection.RandomizedSearchCV
- •

Using the cross_val_score API.

```
print("USING A DECISION TREE WITH cross_val_score (MEAN ACCURACY)...")
X = X.drop(['Name', 'Sex', 'Age', 'Ticket', 'Cabin', 'Embarked'], axis=1)
clf = DecisionTreeClassifier(criterion = 'gini', max_depth = 10, random_state=2021)
scores = cross_val_score(clf, X, y, cv=10)
print(scores)
print("RESULT: %0.2f accuracy with a standard deviation of %0.2f" % (scores.mean(), scores.std()))

USING A DECISION TREE WITH cross_val_score (MEAN ACCURACY)...
[0.58888889 0.61797753 0.52808989 0.50561798 0.61797753 0.70786517
0.70786517 0.70786517 0.59550562 0.74157303]
RESULT: 0.63 accuracy with a standard deviation of 0.08
```

Or iterating manually with K-fold...

```
1.1.1
Iterating manually (with K-fold, Repeated K-fold, Leave One Out, Shuffle Split, Stratified k-fold, TimeSeriesSplit, ...)
print("USING A DECISION TREE WITH MANUAL ITERATION (KFold) and obtaining confusion matrix...")
from sklearn.model selection import KFold
scores = []
kf = KFold(n splits=10)
for train, test in kf.split(X):
    clf.fit(X.loc[train,:], y.loc[train,:])
    score = clf.score(X.loc[test,:], y.loc[test,:])
    scores.append(score)
    y predicted = clf.predict(X.loc[test,:])
    print("Confusion Matrix:")
    print(confusion matrix(y.loc[test,:], y predicted))
    print(score)
print("RESULT: %0.2f accuracy with a standard deviation of %0.2f" % (np.mean(scores), np.std(scores)))
USING A DECISION TREE WITH MANUAL ITERATION (KFold) and obtaining confusion matrix...
Confusion Matrix:
[[45 6]
 [27 12]]
0.6333333333333333
Confusion Matrix:
[[33 36]
[ 8 12]]
0.5056179775280899
Confusion Matrix:
[[38 17]
[19 15]]
0.5955056179775281
RESULT: 0.65 accuracy with a standard deviation of 0.06
```

Hands On

