University of Minho
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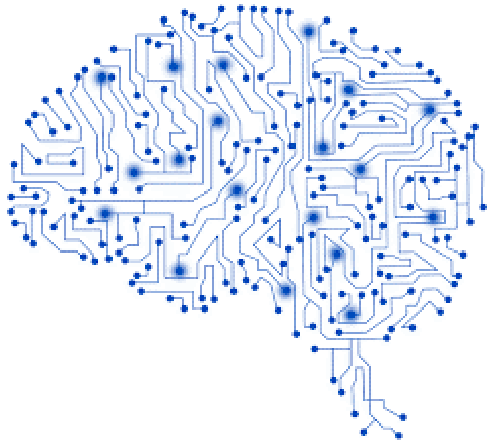

Dados e Aprendizagem Automática

Quality Metrics and Model Validation

DAA @ MEI-1º/MiEI-4º – 1º Semestre

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Part II

Contents

Decision Trees

A Machine Learning Algorithm

We will start with **Decision Trees**.

- A Decision Tree is a model that predicts the value of a target feature:
  - It is a hierarchical graph (a tree)
  - Each branch represents a selection among a set of alternatives
  - Each leaf node represents a class

Decision Tree Classifier

A **Decision Tree Classifier** 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

Decision Tree Regressor

On the other side, a **Decision Tree Regressor** is used for regression problems (the target feature is real/continuous):

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

Decision Tree Classifier

Implementing a Decision Tree Classifier: Data Loading

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

```
'''
Load CSV
'''
df = pd.read_csv('titanic_dataset.csv')
```

```
'''
Inspect dataset
'''
df.columns
```

```
Index(['PassengerId', 'Survived', 'Pclass', 'Name', 'Sex', 'Age', 'SibSp',
       'Parch', 'Ticket', 'Fare', 'Cabin', 'Embarked'],
      dtype='object')
```

Implementing a Decision Tree Classifier: Defining X and y

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

- **X** is typically used to identify the **input**
- **y** to identify the **target**

```
X = df.drop(['Survived'], axis=1)      #input features - everything except the Survived feature
y = df['Survived'].to_frame()          #target feature
```

```
X
```

	PassengerId	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	C
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

891 rows × 11 columns

```
y
```

	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:

Amount of data for testing 25%

Random seed

```
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))
```

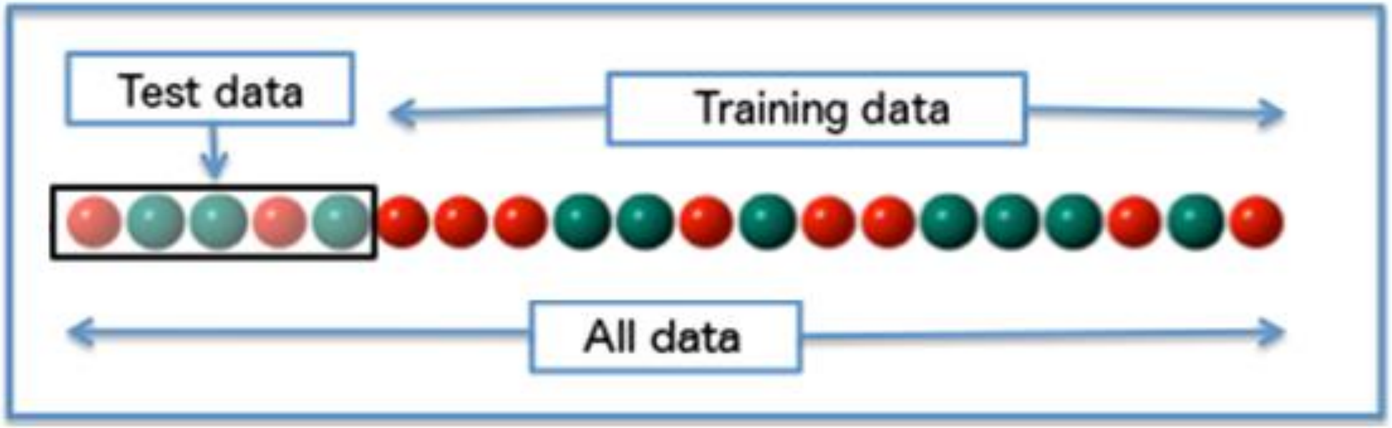
```
The shape of X (891, 11). X_train has shape (668, 11) while X_test has shape (223, 11)
```

```
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)
```

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**:

```
clf = DecisionTreeClassifier(random_state=2021)
```

```
clf.fit(X_train, y_train)
```

Implementing a Decision Tree Classifier: Model Fitting

Ups!

```
clf = DecisionTreeClassifier(random_state=2021)
```

```
clf.fit(X_train, y_train)
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
/tmp/ipykernel_3833/2168925757.py in ?()
      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)
```

```
clf.fit(X_train, y_train)
```

```
▾ DecisionTreeClassifier
DecisionTreeClassifier(random_state=2021)
```

Implementing a Decision Tree Classifier: Predictions

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):

```
predictions = clf.predict(X_test)
predictions
```

```
array([0, 1, 0, 0, 0, 0, 1, 1, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0,
       1, 1, 0, 1, 0, 0, 1, 1, 1, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0,
       1, 0, 0, 0, 1, 0, 0, 1, 1, 1, 1, 0, 1, 0, 0, 1, 1, 0, 1, 0, 1, 0,
       0, 1, 0, 0, 1, 1, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 1, 1, 0, 0, 1, 1,
       0, 0, 1, 1, 1, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 1, 1, 0, 0, 1, 0, 0, 1, 0, 1, 0, 0, 1, 0, 1, 1, 0, 0, 0, 0, 0,
       0, 1, 1, 0, 0, 1, 0, 1, 1, 1, 0, 0, 1, 1, 1, 0, 1, 1, 0, 1, 0, 1,
       0, 0, 0, 0, 1, 0, 1, 0, 0, 1, 0, 0, 0, 1, 0, 0, 1, 0, 1, 0, 0, 1,
       1, 0, 0, 0, 0, 0, 1, 1, 0, 1, 1, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0,
       1, 1, 1, 1, 0, 0, 0, 1, 0, 0, 1, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0,
       1, 1, 0])
```

```
print(y_test.values.shape)
```

```
(223, 1)
```

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

Quality Metrics

Quality Metrics and Model Evaluation

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 Mean Absolute Error, Mean Squared Error, Accuracy, F1-Score, ... There are many!

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

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.root_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
from sklearn.metrics import root_mean_squared_error
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np

from sklearn.model_selection import cross_val_score
```

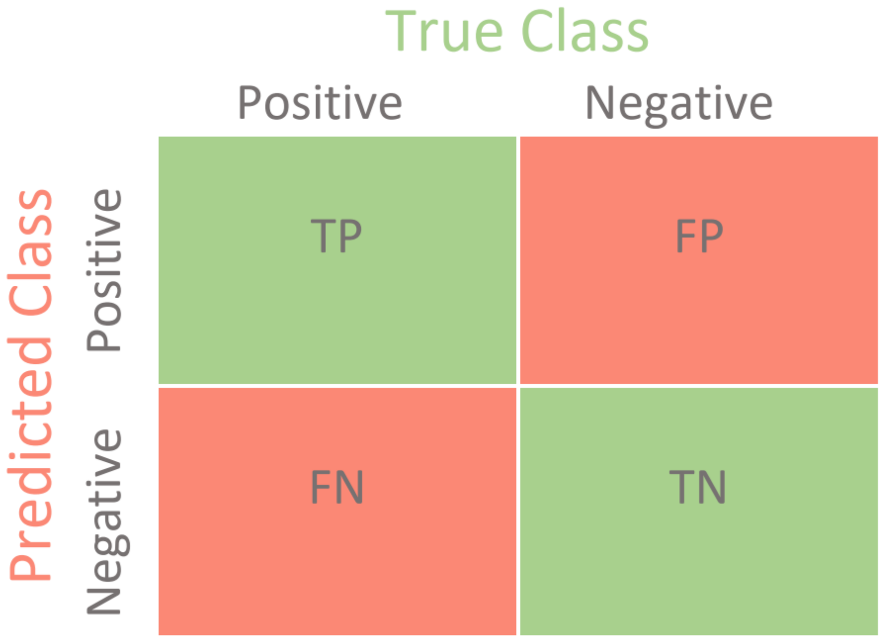
Quality Metrics

Some examples:

- Confusion Matrix
- Accuracy
- Precision
- Recall
- ROC
- AUC
- F1 Score
- Fβ 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.



Classification Models: Accuracy

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

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

		True Class	
		Positive	Negative
Predicted Class	Positive	TP	FP
	Negative	FN	TN

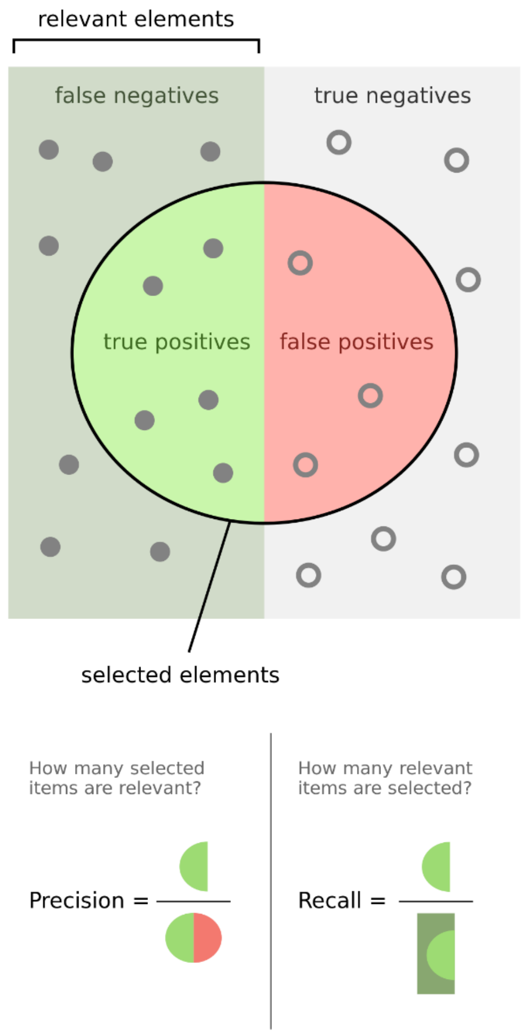
Classification Models: Precision and Recall

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

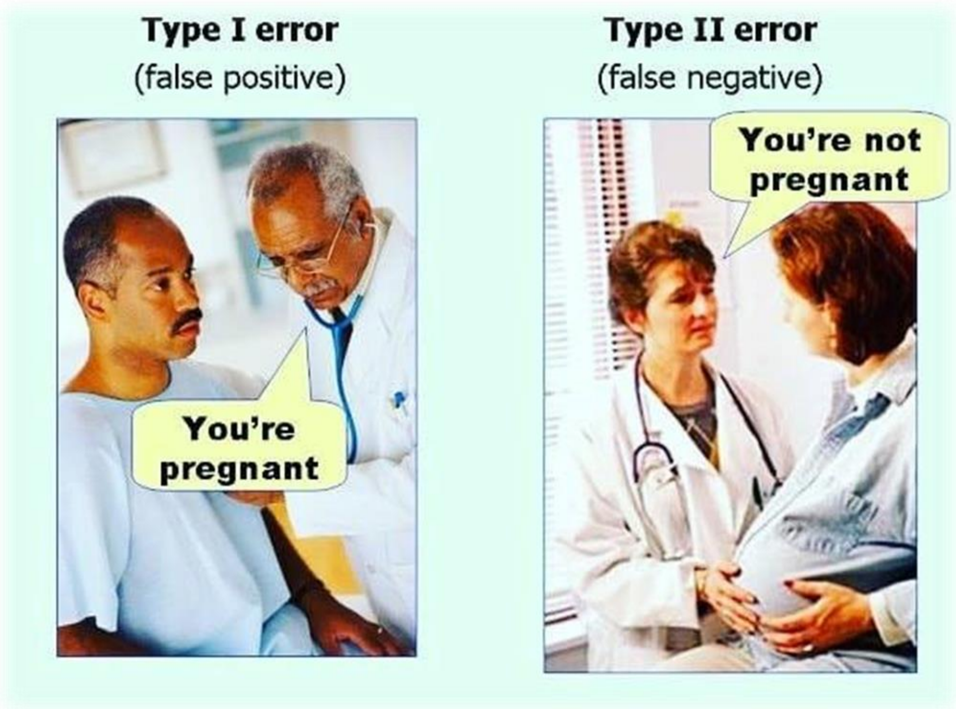
$$Precision = \frac{TP}{TP + FP}$$

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

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



Classification Models: Precision and Recall



Confusion Matrix-based Metrics

Obtaining the **confusion matrix** is as simple as:

```
confusion_matrix(y_test, predictions)
```

```
array([[96, 39],
       [43, 45]])
```

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

```
accuracy_score(y_test, predictions)
```

```
0.6322869955156951
```

```
precision_score(y_test, predictions)
```

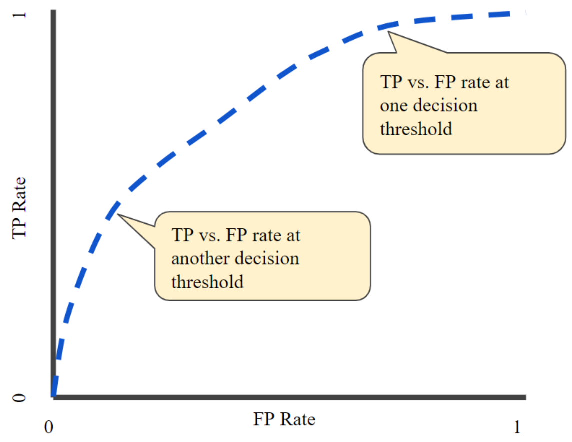
```
0.5357142857142857
```

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

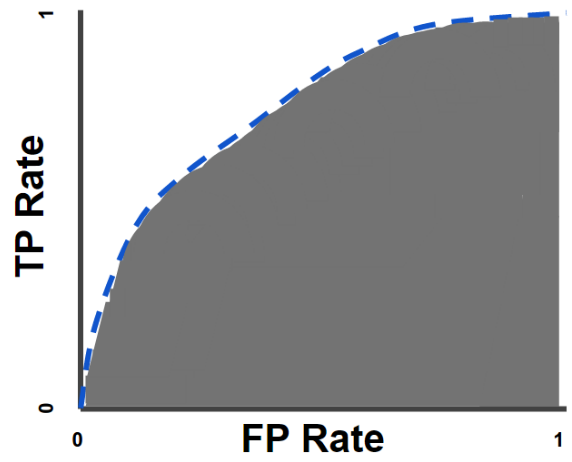
```
0.5113636363636364
```

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.



(https://towardsdatascience.com/receiver-operating-characteristic-curves-demystified-in-python-bd531a4364d0)

ROC and AUC

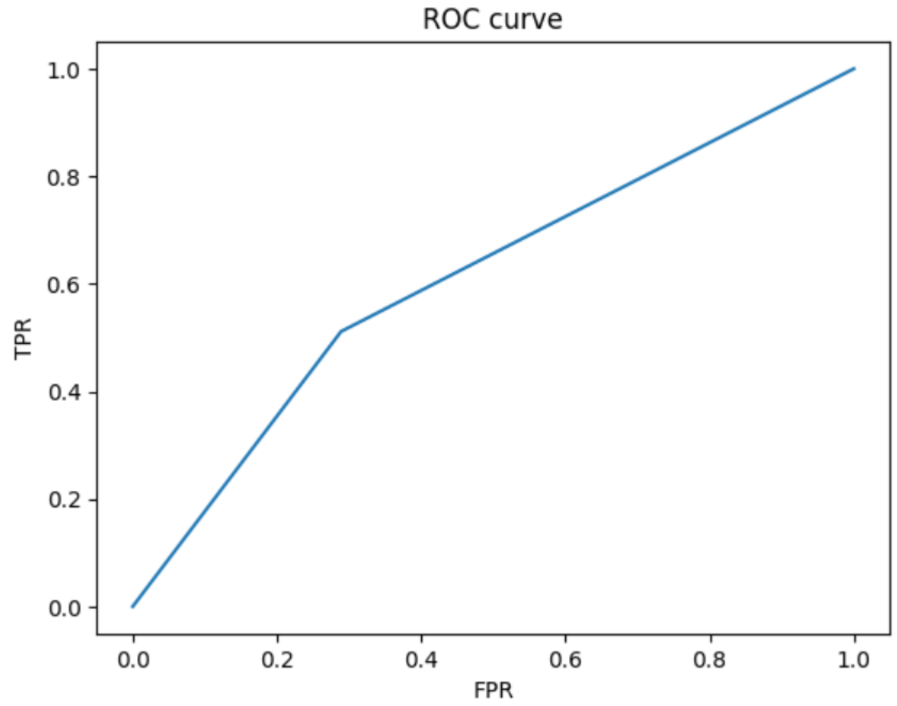
As for the **ROC** and the **AUC**:

```
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 β=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 $\mathbf{F_1}$ and $\mathbf{F_\beta}$ **Score**:

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

```
0.5232558139534884
```

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

```
0.5306603773584905
```

Decision Tree Regressor

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:

```
X = df.drop(['Fare'], axis=1)      #input features - everything except the Fare feature
y = df['Fare'].to_frame()          #target feature
```

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

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.25, random_state=2021)
```

```
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:

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

```
▾          DecisionTreeRegressor
DecisionTreeRegressor(random_state=2021)
```

```
#obtaining predictions
predictions = clf.predict(X_test)
predictions
```

```
array([ 18.7875,   7.8958,  10.5   ,  27.9   ,  34.375 ,  24.15  ,
       211.5   ,   7.7417,  12.35  ,   7.2292,   7.2292,  52.    ,
        15.5   ,  18.7875,  13.    ,   8.6625,   8.05  ,  52.    ,
         8.6625,  35.5   ,  76.2917,  15.5   ,   7.6292,   8.4042,
         8.6625,   7.125 ,   7.775 ,   7.65  ,  93.5   ,  26.    ,
         7.8792,   8.6625,  39.6875,  16.1   , 113.275 ,  12.35  ,
```

We now have fare predictions for the test set (and <u>we know the actual fare value as it is stored in the **y_test** variable</u>). How do we **evaluate** our regression model?

Quality Metrics

Mean Absolute Error

Mean Absolute Error (**MAE**) 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 $\boldsymbol{y_j}$ and $\hat{y}_{\boldsymbol{j}}$ are the actual observation and the predicted value, respectively.

Mean Squared Error

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

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

Where **n** is the number of observations, and $\boldsymbol{y_j}$ and $\hat{y}_{\boldsymbol{j}}$ are the actual observation and the predicted value, respectively.

Root Mean Squared Error

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

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

Where **n** is the number of observations, and $\boldsymbol{y_j}$ and $\hat{y}_{\boldsymbol{j}}$ are the actual observation and the predicted value, respectively.

Regression Quality Metrics

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

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

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

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

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

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

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

#	Error	|Error|	$Error^2$
1	1	1	1
2	-1	1	1
3	3	3	9
4	3	3	9

MAE	MSE	RMSE
2	5	2.24

#	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	25	5

Regression Quality Metrics

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

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

```
14.68592556053812
```

```
mean_squared_error(y_test, predictions)
```

```
1399.7722041242152
```

```
root_mean_squared_error(y_test, predictions)
```

```
37.41352969347072
```

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

Model Evaluation

Model Validation

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?

Model Validation

- 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?

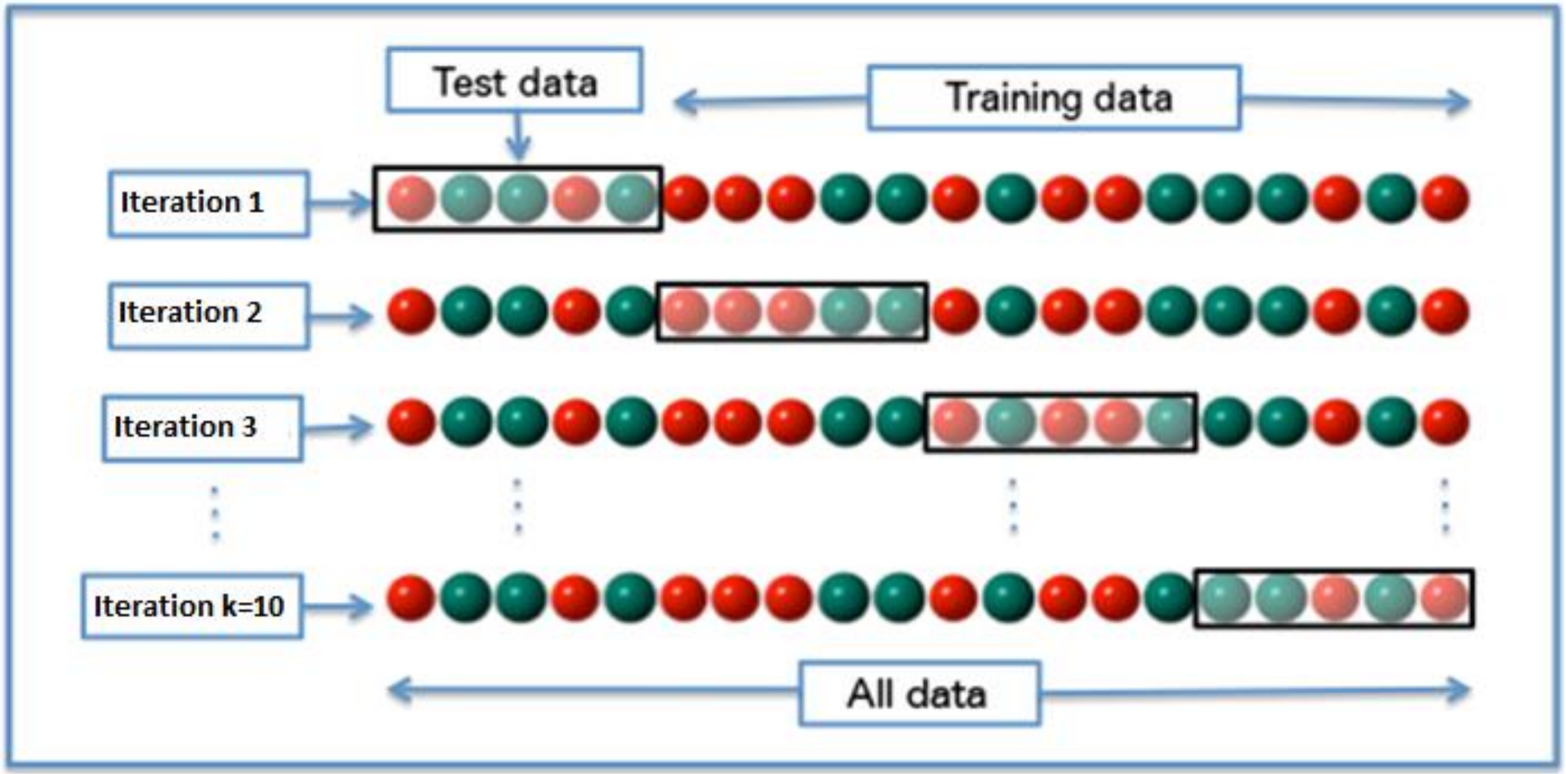
A **greater number of folds** will lead to a **better error estimate** of the model, a **lower bias** and **less overfitting**. However, it comes with a **higher computational cost**!

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**!

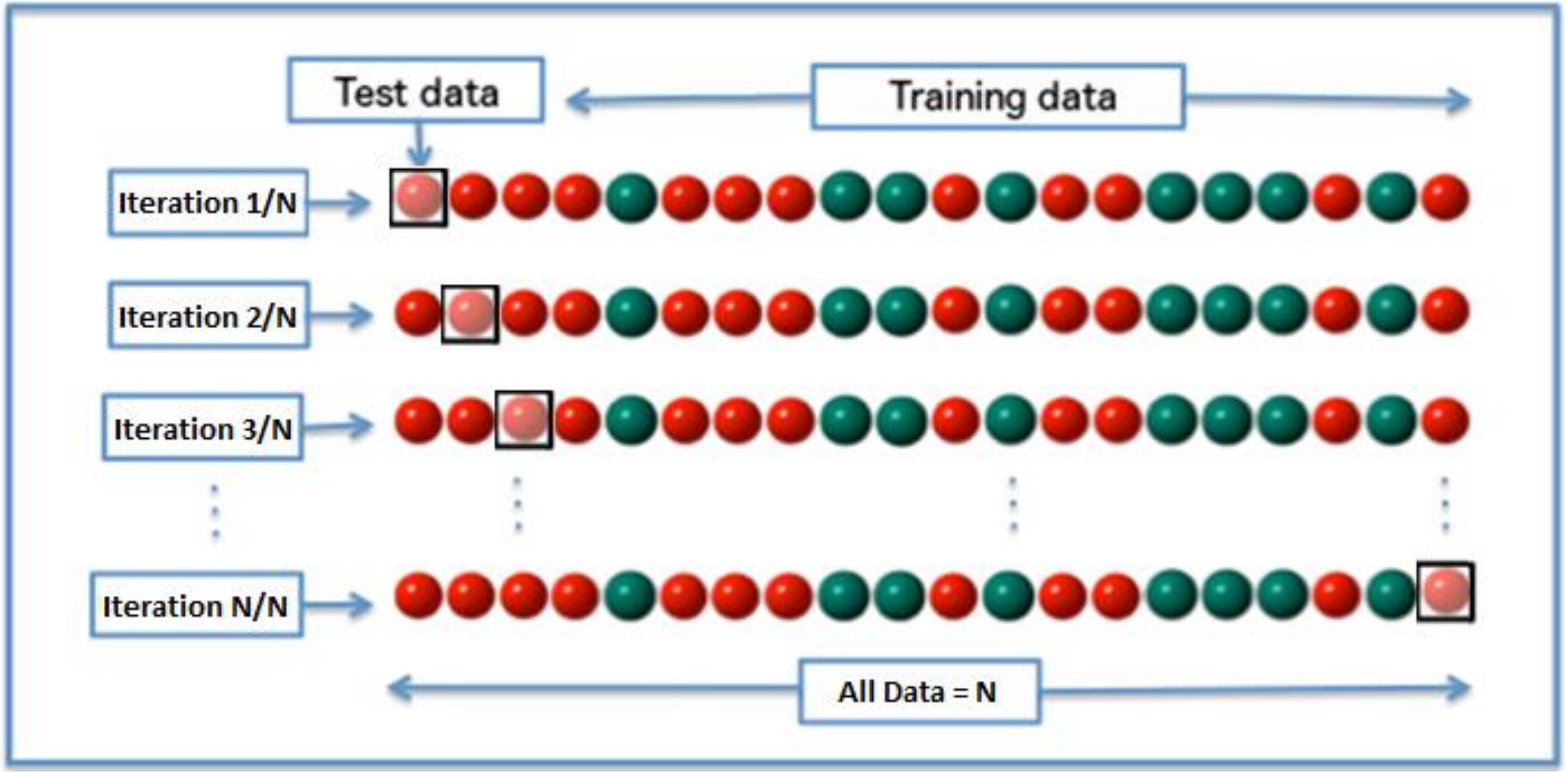
Row ID	D Error in %	I Size of Test Set	I Error Count
fold 0	38.281	128	49
fold 1	35.156	128	45
fold 2	44.531	128	57
fold 3	42.969	128	55
fold 4	42.969	128	55
fold 5	41.406	128	53
fold 6	41.406	128	53
fold 7	40.625	128	52
fold 8	41.406	128	53
fold 9	42.52	127	54

k-fold Cross Validation



Usually, **k=10**

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**.

Model Validation

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
```

…

Model Validation

Using the cross_val_score API:

```
'''
Load CSV
'''
df = pd.read_csv('titanic_dataset.csv')
```

```
#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
```

```
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()))
```

10 folds!

```
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
```

Model Validation

Or iterating manually with K-fold:

```
print("USING A DECISION TREE WITH MANUAL ITERATION (KFold) and obtaining confusion matrix...")
from sklearn.model_selection import KFold
clf = DecisionTreeClassifier(criterion='gini', max_depth=10, random_state=2021)
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:
```

```
Confusion Matrix:
[[41 15]
 [14 19]]
0.6741573033707865
RESULT: 0.65 accuracy with a standard deviation of 0.06
```

Hands On