Supervised Learning

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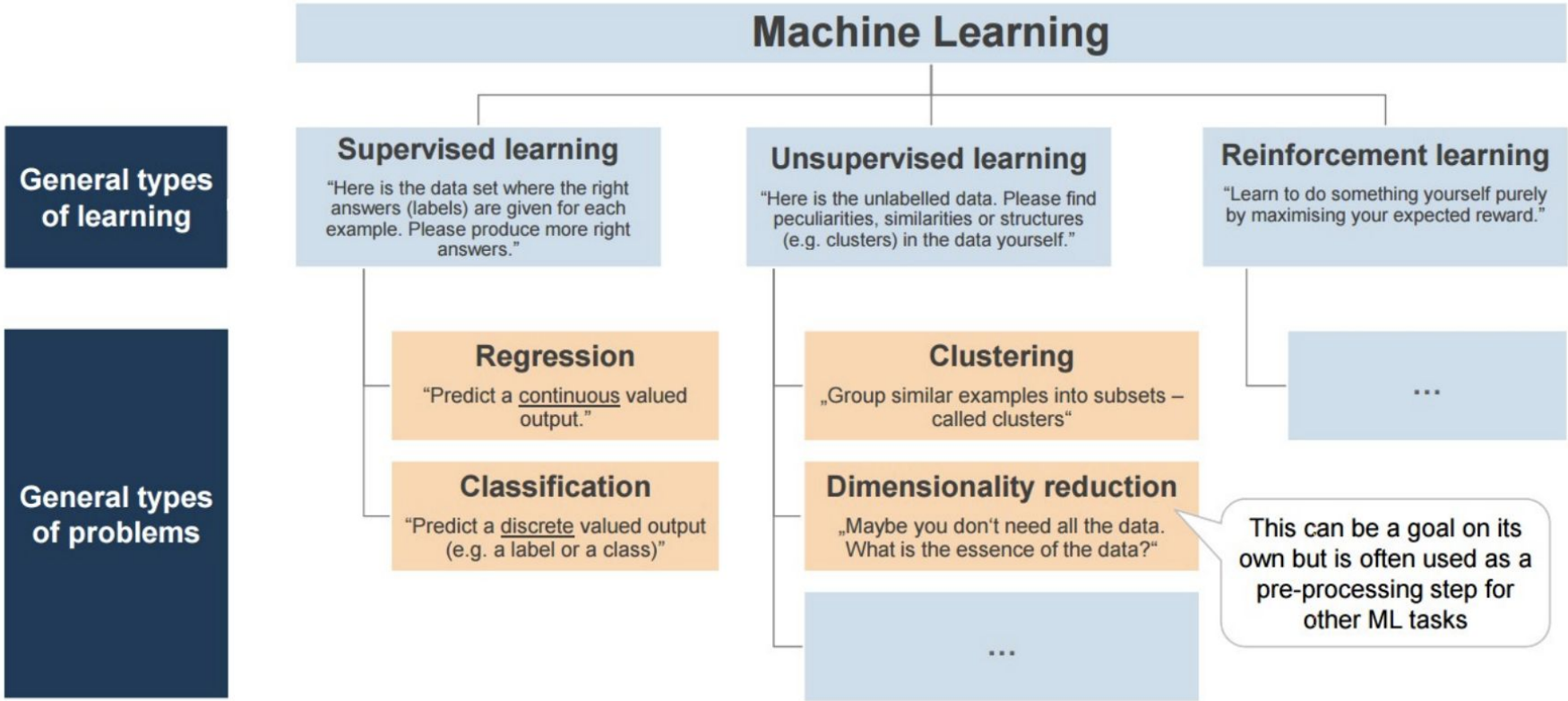

Machine Learning
General types of learning
Supervised learning
"Here is the data set where the right answers (labels) are given for each example. Please produce more right answers."
Unsupervised learning
"Here is the unlabelled data. Please find peculiarities, similarities or structures (e.g. clusters) in the data yourself."
Reinforcement learning
"Learn to do something yourself purely by maximising your expected reward."
General types of problems
Regression
"Predict a continuous valued output."
Classification
"Predict a discrete valued output (e.g. a label or a class)"
Clustering
„Group similar examples into subsets – called clusters"
Dimensionality reduction
„Maybe you don't need all the data. What is the essence of the data?"
...
...
This can be a goal on its own but is often used as a pre-processing step for other ML tasks

Agenda

Machine Learning:

- Features
- Model
- Metrics

And as well:

- Model Interpretability
- Saving Models

What is supervised learning ?

Supervised Learning requires **Labelled Training Data**:

- Pairs of vectors (Input,Output)

Then a relationship between input and output is built. The results is a:

- Regressor: output is a Number
- Classifier: output is a Class

Which families of relationships ?

Regression:

- Linear Regression
- k neighbor Regressor
- Decision Tree

Classification:

- Logistic Regression
- k neighbor Classifier
- Support Vector Machine
- Decision Tree Classifier

Metric: Evaluation of Performance

Regression:

- RMSE
- MAE and MAPE
- Correlation and Bias

Classification:

- Accuracy
- Precision and Recall
- AUC Curve

Regression

Problem Statement

We would like to predict the price of a house. We have labeled data with:

- Input: Area of the house
- Output: Price of the house

Predict house prices.

Preparing the data

```
# Input

X = df[['TotalSF']] # pandas DataFrame


# Label

y = df["SalePrice"] # pandas Series
```

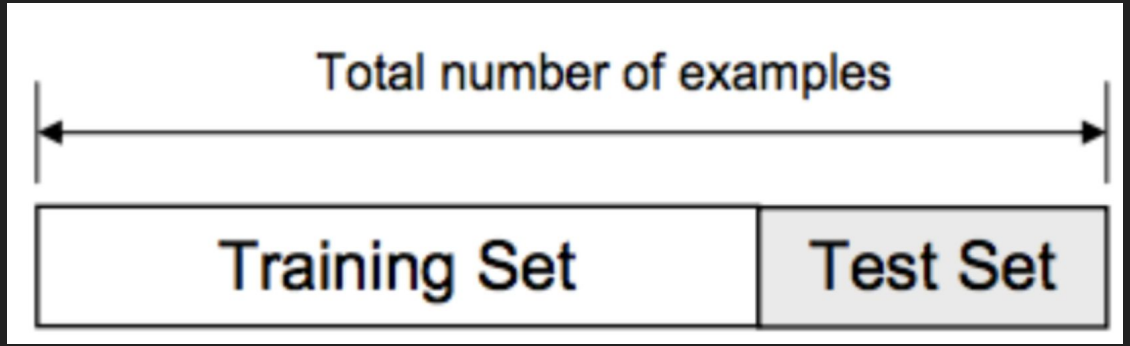
Linear Regression with Sklearn

```
# Load the library
from sklearn.linear_model import LinearRegression

# Create an instance of the model
reg = LinearRegression()

# Fit the regressor
reg.fit(X,y)

# Do predictions
reg.predict([[2540],[3500],[4000]])
```

How good is my regressor ?

In order to evaluate the regressor we just created, we would need to compare the predictions with real actual values. We are TESTING the regressor.

We divide our labeled original data into 2 sets: **Training** and **Testing Sets**



Train-Test Split in Sklearn

```
# Load the library

from sklearn.model_selection import train_test_split

# Create 2 groups each with input and labels

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.10)

# Fit only with training data

reg.fit(X_train,y_train)
```

Metrics: MAE and MAPE

MAE is the sum of the absolute values of the error:

$$\frac{\sum_{i=1}^{n} |y_i - x_i|}{n} = \frac{\sum_{i=1}^{n} |e_i|}{n}$$

MAPE is almost the same but gives the percentage of the absolute value of error

$$\frac{\sum_{i=1}^{n} |y_i - x_i|}{n|y_i|} = \frac{\sum_{i=1}^{n} |e_i|}{n|y_i|}$$

MAE in sklearn

```
# Load the scorer

from sklearn.metrics import mean_absolute_error

# Use against predictions

mean_absolute_error(reg.predict(X_test),y_test)
```

MAPE is not in Sklearn, so we implement ourselves

```
np.mean(np.abs(reg.predict(X_test)-y_test)/y_test)
```

k Nearest Neighbors

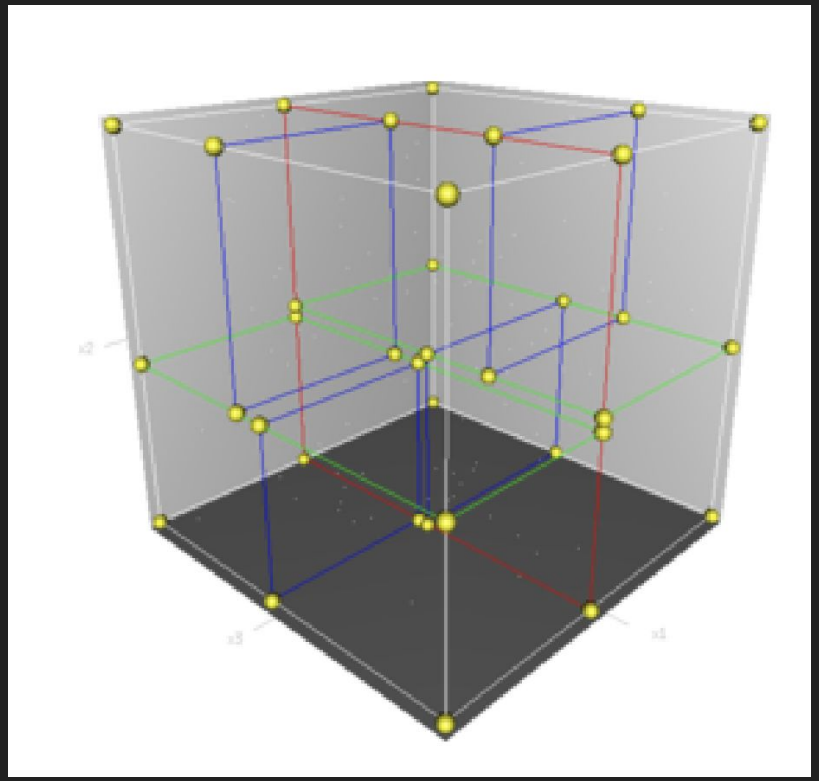
k Nearest Neighbors predicts by taking the k nearest neighbors to the input from the training data, and then combines the labels of each.

It requires that the dataset has a **DISTANCE.**

No Training Phase :) BUT it keeps all the data

Warning: if it is found that two neighbors, neighbor k+1 and k, have identical distances but different labels, the results will depend on the ordering of the training data.

k Nearest Neighbors: Data Partition



k Nearest Neighbors: Parameters

k: Number of neighbors

weight: Way to combine the label of the nearest point

- **Uniform: All the same**
- **Distance: Weighted Average per distance**
- **Custom: Weighted Average provided by user**

partition: Way to partition the training dataset (ball_tree, kd_tree, brute)

k Nearest Neighbors in Sklearn

```
# Load the library

from sklearn.neighbors import KNeighborsRegressor

# Create an instance

regk = KNeighborsRegressor(n_neighbors=2)

# Fit the data

regk.fit(X,y)
```

Metric: RMSE

RMSE **penalizes more high values** of error

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (y_i - x_i)^2}{n}}$$

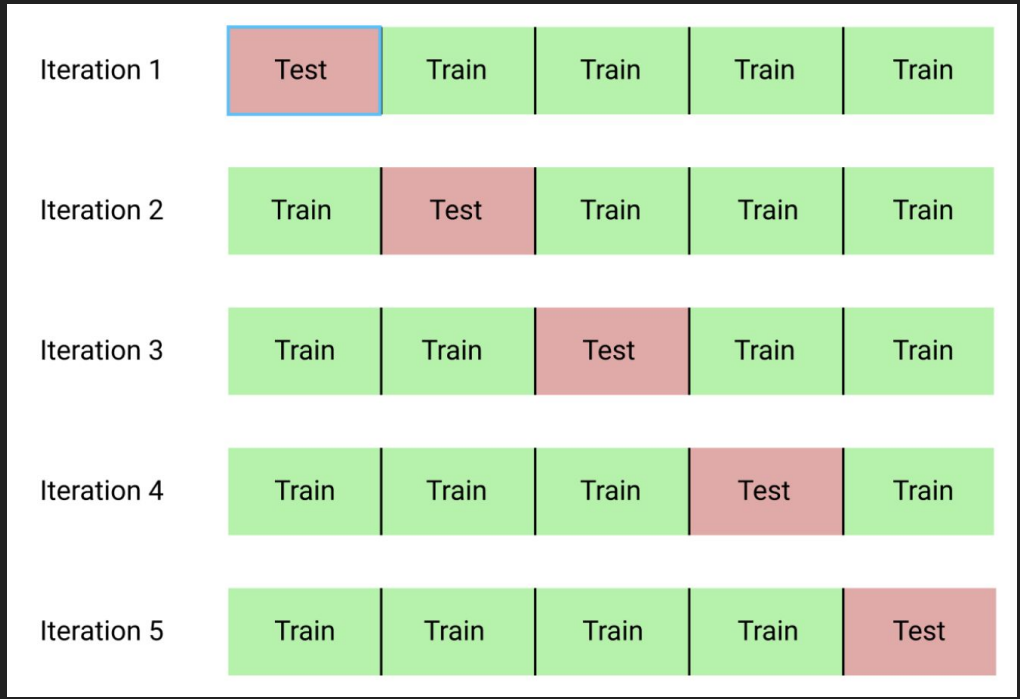
RMSE in Sklearn

```
# Load the scorer

from sklearn.metrics import mean_squared_error

# Use against predictions (we must calculate the square root of the MSE)

np.sqrt(mean_squared_error(reg.predict(X_test),y_test))
```

Cross Validation

The dataset is split into n random parts. Then we iterate by:

- Training with n-1 chunks
- Test with the remainder
- We then can calculate mean or variance of the error.



Cross Validation in Sklearn

```
# Load the library

from sklearn.model_selection import cross_val_score

# We calculate the metric for several subsets (determine by cv)

# With cv=5, we will have 5 results from 5 training/test

cross_val_score(reg,X,y,cv=5,scoring="neg_mean_squared_error")
```

Testing Parameters: GridSearchCV

We could then try to find the best parameters by testing all of the combinations of them. We test a GRID of parameters.

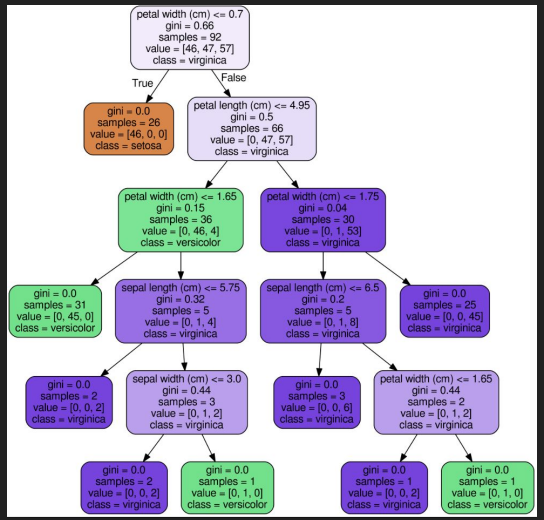
```
from sklearn.model_selection import GridSearchCV

from sklearn.neighbors import KNeighborsRegressor

reg_test = GridSearchCV(KNeighborsRegressor(),

                        param_grid={"n_neighbors":np.arange(3,50)})

# Fit will test all of the combinations

reg_test.fit(X,y)
```

Testing Parameters: GridSearchCV

```
# Fit will test all of the combinations

reg_test.fit(X,y)

# Best estimator and best parameters

reg_test.best_score_

reg_test.best_estimator_

reg_test.best_params_
```

Decision Tree

A decision tree is a structure that includes a root node, branches, and leaf nodes. Each internal node denotes a test on an attribute, each branch denotes the outcome of a test, and each leaf node holds a class label. The topmost node in the tree is the root node.



Decision Tree: Building homogeneous partitions

- Start at the training dataset
- For each feature:
  - Split in 2 partitions
  - Calculate the purity/homogeneity gain
- Keep the feature split with the best gain
- Repeat for the 2 new partitions

Homogeneity gain is calculated with the variance (regression) or entropy (classification).

Decision Tree: Main Parameters

Max_depth: Number of Splits

Min_samples_leaf: Minimum number of observations per leaf

Decision Tree in Sklearn

```
# Load the library

from sklearn.tree import DecisionTreeRegressor

# Create an instance

regd = DecisionTreeRegressor(max_depth=3)

# Fit the data

regd.fit(X,y)
```

Metric: Correlation

Correlation measures the correlation between the predictions and the real value.

```
# Direct Calculation
np.corrcoef(reg.predict(X_test),y_test)[0][1]


# Custom Scorer
from sklearn.metrics import make_scorer
def corr(pred,y_test):
      return np.corrcoef(pred,y_test)[0][1]
# Put the scorer in cross_val_score
cross_val_score(reg,X,y,cv=5,scoring=make_scorer(corr))
```

Metric: Bias

Bias is the average of errors.

```
# Direct Calculation
np.mean(reg.predict(X_test)-y_test)

# Custom Scorer
from sklearn.metrics import make_scorer
def bias(pred,y_test):
      return np.mean(pred-y_test)
# Put the scorer in cross_val_score
cross_val_score(reg,X,y,cv=5,scoring=make_scorer(bias))
```

Drawing the Decision Tree

```
from IPython.display import Image

from sklearn.tree import export_graphviz

import pydotplus

dot_data = StringIO()

export_graphviz(dtree, out_file=dot_data,filled=True, rounded=True,

                special_characters=True)

graph = pydotplus.graph_from_dot_data(dot_data.getvalue())

Image(graph.create_png())
```

Bias-variance tradeoff

We must find a compromise between two sources of error:

The **bias** is error from erroneous assumptions in the learning algorithm. High bias can cause an algorithm to miss the relevant relations between features and target outputs (**underfitting**).

The **variance** is error from sensitivity to small fluctuations in the training set. High variance can cause **overfitting**: modeling the random noise in the training data, rather than the intended outputs.

Classification

Problem Statement

Determine if the car should go fast or slow according to the bumpiness and slope of the route.

Logistic Regression in sklearn

```
# Load the library

from sklearn.linear_model import LogisticRegression

# Create an instance of the classifier

clf=LogisticRegression()

# Fit the data

clf.fit(X,y)
```

Metric: Accuracy

```
# With Metrics

from sklearn.metrics import accuracy_score

accuracy_score(y_test,clf.predict(X_test))


# Cross Validation

cross_val_score(clf,X,y,scoring="accuracy")
```

k nearest neighbor (Same Parameters)

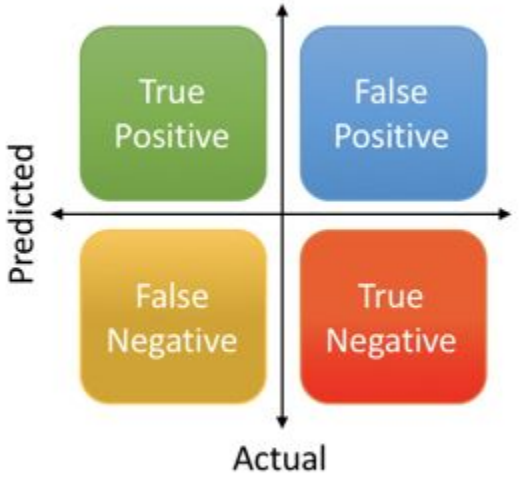
```
# Load the library
from sklearn.neighbors import KNeighborsClassifier
# Create an instance
regk = KNeighborsClassifier(n_neighbors=2)
# Fit the data
regk.fit(X,y)
```

Metric: Precision and Recall

$$\textbf{Precision} = \frac{\text{True Positive}}{\text{Actual Results}} \quad \text{or} \quad \frac{\text{True Positive}}{\text{True Positive + False Positive}}$$

$$\textbf{Recall} = \frac{\text{True Positive}}{\text{Predicted Results}} \quad \text{or} \quad \frac{\text{True Positive}}{\text{True Positive + False Negative}}$$

$$\textbf{Accuracy} = \frac{\text{True Positive + True Negative}}{\text{Total}}$$



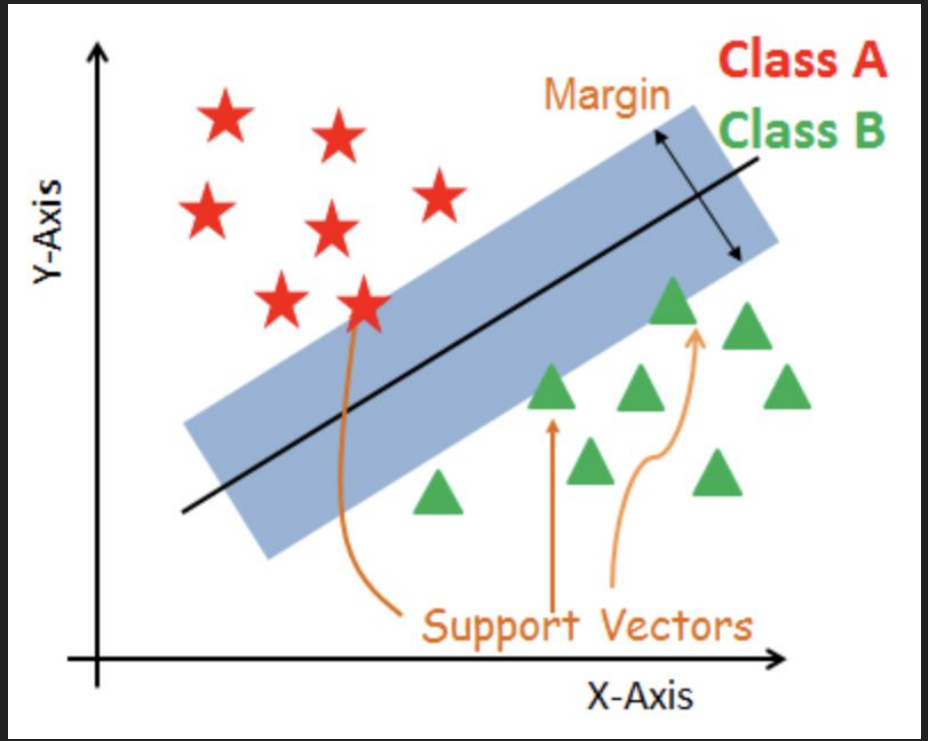
Metric: Precision and Recall

```
# Metrics

from sklearn.metrics import precision_score, recall_score

from sklearn.metrics import confusion_matrix, classification_report

precision_score(y_test,clf.predict(X_test))

classification_report(y_test,clf.predict(X_test))


# Cross Validation

cross_val_score(clf,X,y,scoring="precision")

cross_val_score(clf,X,y,scoring="recall")
```

Support Vector Machine

Classes are separated by a line.

(See joined notebook)



Support Vector Machines: Main Parameters

C: Sum of Error Margins

kernel:

- **linear: line of separation**
- **rbf: circle of separation**
  - **Additional param gamma: Inverse of the radius**
- **poly: curved line of separation**
  - **Additional param degree: Degree of the polynome**

Support Vector Machine in Sklearn

```
# Load the library

from sklearn.svm import SVC

# Create an instance of the classifier

clf = SVC(kernel="linear",C=10)

# Fit the data

clf.fit(X,y)
```

Decision Tree in Sklearn

```
# Import library

from sklearn.tree import DecisionTreeClassifier

# Create instance

clf = DecisionTreeClassifier(min_samples_leaf=20,max_depth=3)

# Fit the data

clf.fit(X,y)
```

Predict Probability

A classifier can not only predict a class. It can also predict the probability of each class.

Probability of first instance being a 0

Probability of first instance being a 1

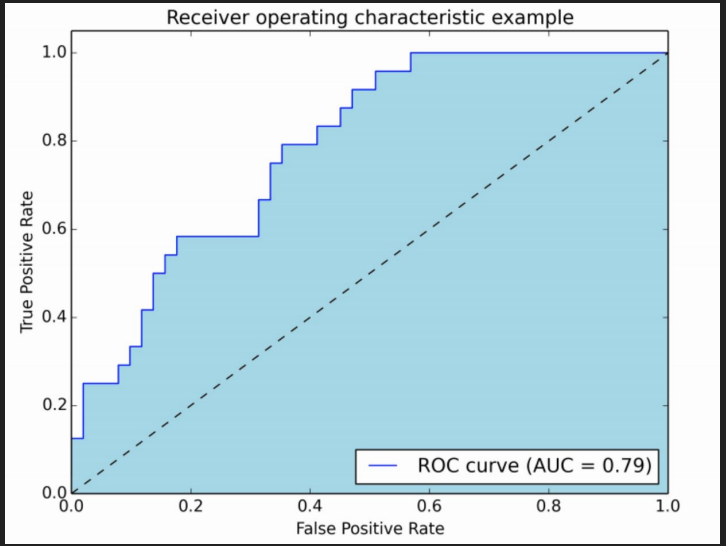
	0	1
0	0.350438	0.649562
1	0.916989	0.083011
2	0.224553	0.775447
3	0.921397	0.078603
4	0.166357	0.833643

Metric: Receiver Operating Characteristic Curve

You can change the threshold and calculate:

- Number of True Positives: Correctly predicted as 1
- Number of False Positives: Incorrectly predicted as 1

The ROC Curve shows how confident your classifier is, with the area under this curve.



ROC Curve in Python

```
# Load the library

from sklearn.metrics import roc_curve



# We chose the target

target_pos = 1 # Or 0 for the other class

fp,tp,_ = roc_curve(y_test,pred[:,target_pos])

plt.plot(fp,tp)
```

AUC metric

```
# Metrics

from sklearn.metrics import roc_curve, auc

fp,tp,_ = roc_curve(y_test,pred[:,1])

auc(fp,tp)



# Cross Validation

cross_val_score(clf,X,y,scoring="roc_auc")
```

Saving and delivering a model

```
clf = DecisionTreeClassifier(max_depth=17)

clf.fit(X,y)

import pickle

pickle.dump(clf,open("modelo.pickle","wb"))



clf_loaded = pickle.load(open("modelo.pickle","rb"))

ndf = pd.read_csv("nuevosind.csv")

clf_loaded.predict(ndf)
```

Latex Formulas

MAE: \frac{\sum_{i=1}^n\left| y_i-x_i\right|}{n} =\frac{\sum_{i=1}^n\left| e_i \right|}{n}

MAPE: \frac{\sum_{i=1}^n\left| y_i-x_i\right|}{n|y_i|} =\frac{\sum_{i=1}^n\left| e_i \right|}{n|y_i|}