

# Supervised Learning

Sebastien Perez  
Toni Almagro

# 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."

#### Regression

"Predict a continuous valued output."

#### Classification

"Predict a discrete valued output (e.g. a label or a class)"

### Unsupervised learning

"Here is the unlabelled data. Please find peculiarities, similarities or structures (e.g. clusters) in the data yourself."

#### 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?"

### Reinforcement learning

"Learn to do something yourself purely by maximising your expected reward."

...

...

This can be a goal on its own but is often used as a pre-processing step for other ML tasks

## General types of problems

# 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)

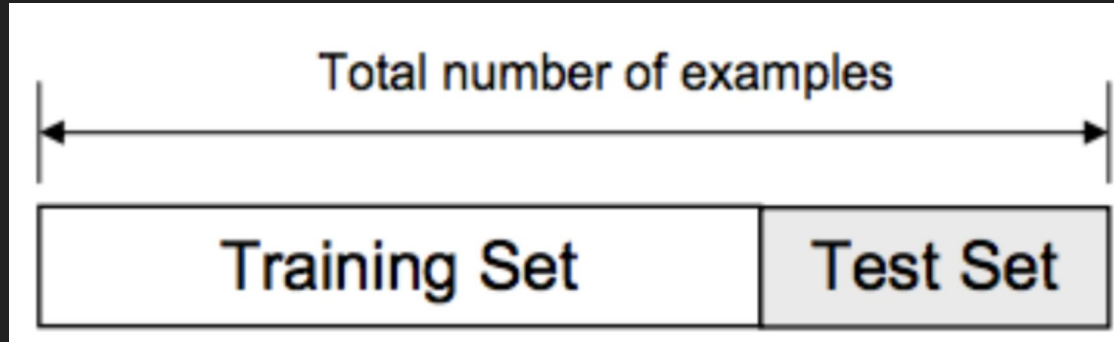
# Do predictions
reg.predict([[2540],[3500],[4000]])
```



# 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.

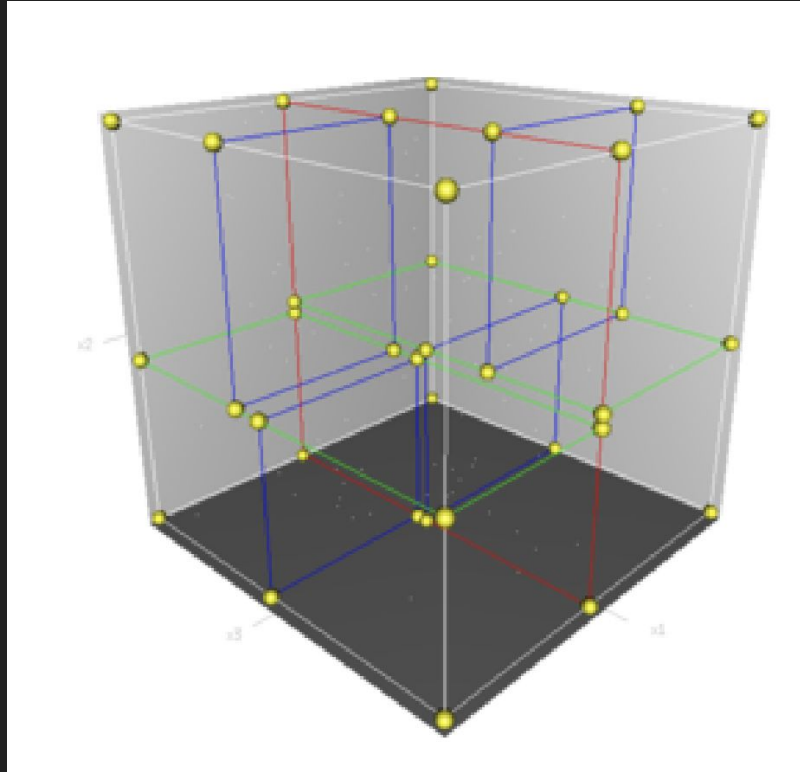
It requires that the dataset has a **DISTANCE**.

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
```

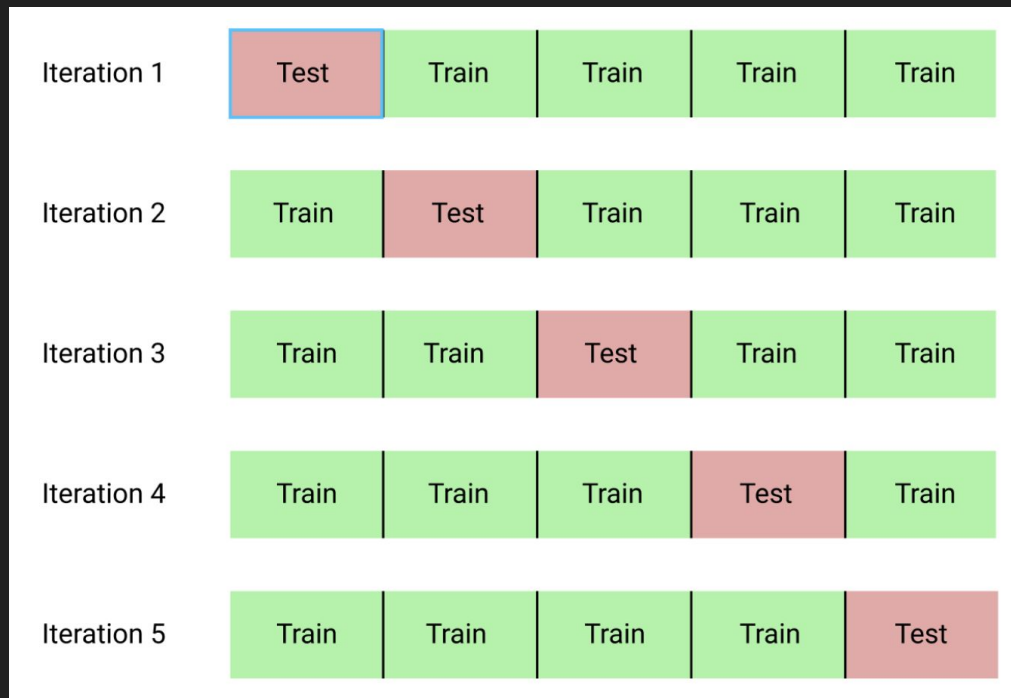
```
# Use against predictions (we must calculate the square root of the MSE)
```

```
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
```

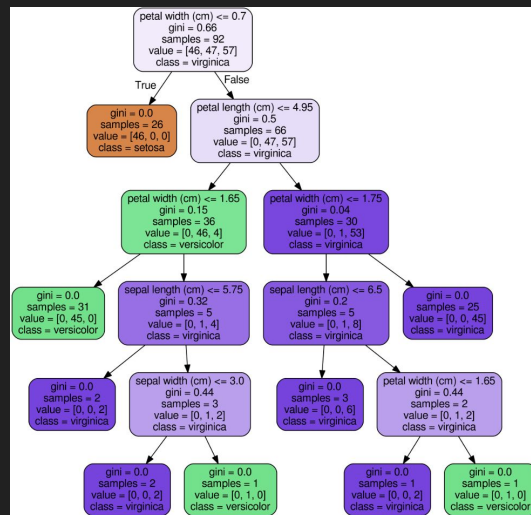
```
reg_test.best_score_
```

```
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)

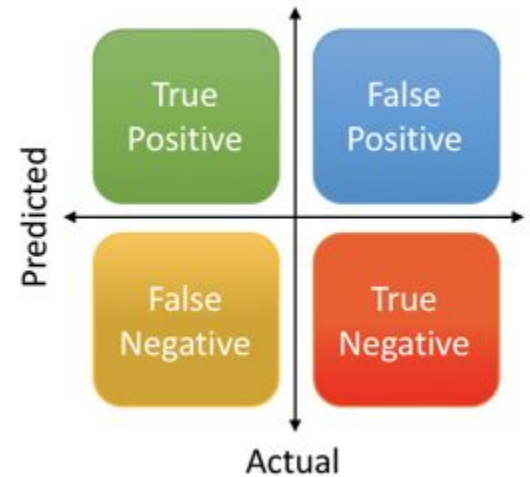
```
# Load the library
from sklearn.neighbors import KNeighborsClassifier
# Create an instance
regk = KNeighborsClassifier(n_neighbors=2)
# Fit the data
regk.fit(X,y)
```

# Metric: Precision and Recall

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

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

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



# 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")
```

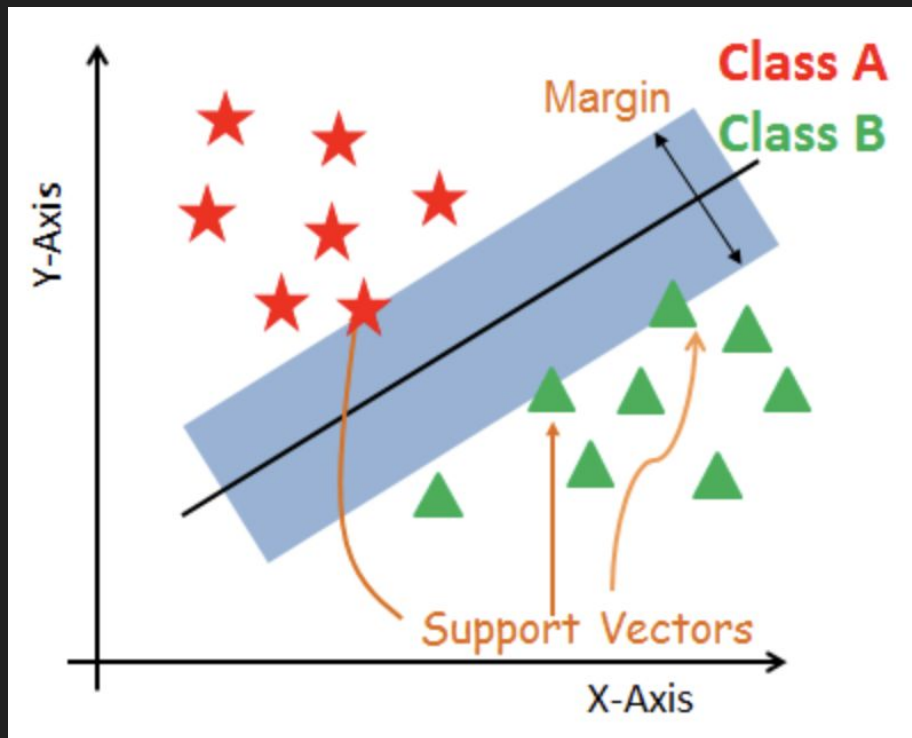
```
cross_val_score(clf,X,y,scoring="recall")
```



# 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



	0	1
<b>0</b>	0.350438	0.649562
<b>1</b>	0.916989	0.083011
<b>2</b>	0.224553	0.775447
<b>3</b>	0.921397	0.078603
<b>4</b>	0.166357	0.833643

Probability of first  
instance being a 1

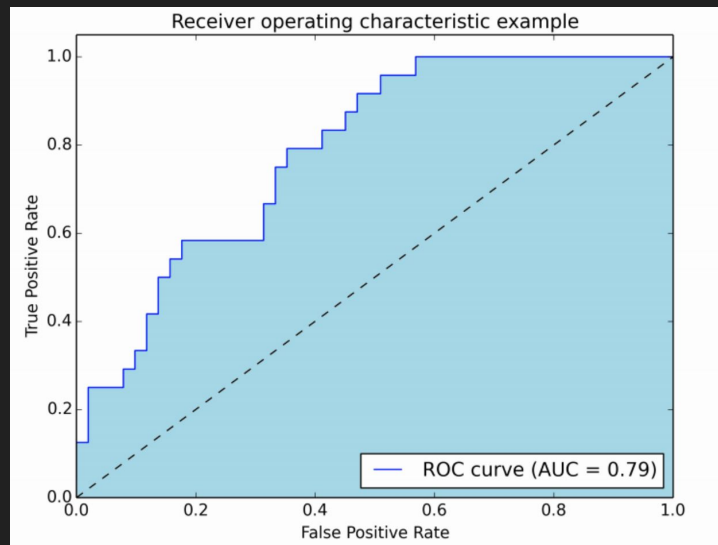


# Metric: Receiver Operating Characteristic Curve

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

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