## dataMining02-data exploration-adults

February 12, 2020

## 1 From UCI Machine Learning Repository

#### 1.1 Adult dataset

This data file does not have a header with column names. Look at the ".names" text file in the Data Folder and use the same procedure used for Iris

Print als the types of the columns using the types attribute

names = ['age', 'workclass', 'fnlwgt', 'education', 'education-num', 'marital-status', 'occupation', 'relationship', 'race', 'sex', 'capital-gain', 'capital-loss', 'hours-per-week', 'native-country', 'high-income']

url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/adult/adult.data'

Load the data in the dataframe df and then show the column types with the .dtypes attribute of a Pandas DataFrame

```
[3]: names =

→ ['age','workclass','fnlwgt','education','education-num','marital-status','occupation'

→,'relationship','race','sex','capital-gain','capital-loss','hours-per-week','native-country

→'high-income']

url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/adult/adult.

→data'

df = pd.read_csv(url, sep = ',', names = names

# , index_col = False # since the first column is integer,

→without this

# it would be interpreted as row label

)
print(df.dtypes)
```

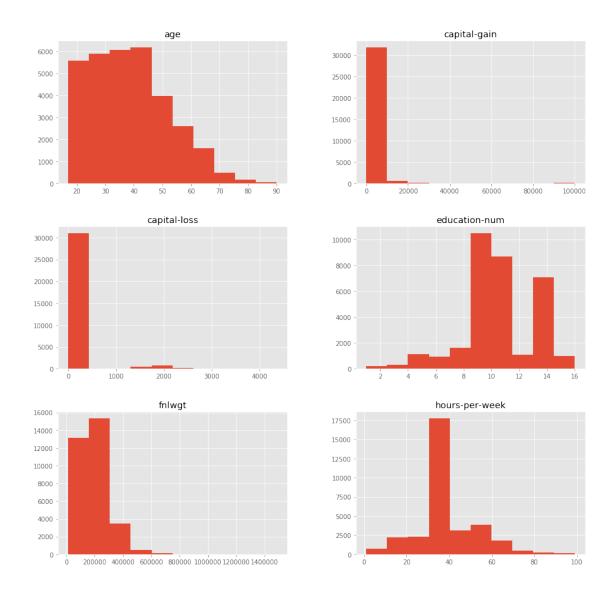
```
int64
age
                   object
workclass
                    int64
fnlwgt
education
                   object
                    int64
education-num
marital-status
                   object
occupation
                   object
relationship
                   object
                   object
race
sex
                   object
capital-gain
                    int64
capital-loss
                    int64
hours-per-week
                    int64
native-country
                   object
high-income
                   object
```

dtype: object

Show the head and then generate the histograms for all the columns

```
[4]: df.head()
[4]:
                                                       education-num
        age
                      workclass
                                 fnlwgt
                                           education
                                  77516
     0
         39
                      State-gov
                                           Bachelors
                                                                  13
     1
         50
              Self-emp-not-inc
                                  83311
                                           Bachelors
                                                                  13
     2
                                                                   9
         38
                                 215646
                                             HS-grad
                        Private
                                                                   7
     3
         53
                        Private
                                 234721
                                                11th
     4
         28
                        Private
                                 338409
                                           Bachelors
                                                                  13
             marital-status
                                       occupation
                                                     relationship
                                                                      race
                                                                                 sex \
     0
              Never-married
                                     Adm-clerical
                                                    Not-in-family
                                                                      White
                                                                                Male
     1
         Married-civ-spouse
                                 Exec-managerial
                                                           Husband
                                                                     White
                                                                                Male
                    Divorced
     2
                               Handlers-cleaners
                                                    Not-in-family
                                                                     White
                                                                                Male
     3
         Married-civ-spouse
                               Handlers-cleaners
                                                           Husband
                                                                     Black
                                                                                Male
         Married-civ-spouse
                                  Prof-specialty
     4
                                                              Wife
                                                                     Black
                                                                              Female
                                     hours-per-week
        capital-gain capital-loss
                                                      native-country high-income
     0
                2174
                                                  40
                                                        United-States
                                                                             <=50K
                                  0
                                                                             <=50K
     1
                    0
                                                  13
                                                        United-States
     2
                    0
                                  0
                                                  40
                                                        United-States
                                                                             <=50K
     3
                    0
                                  0
                                                  40
                                                        United-States
                                                                             <=50K
     4
                    0
                                   0
                                                  40
                                                                 Cuba
                                                                             <=50K
```

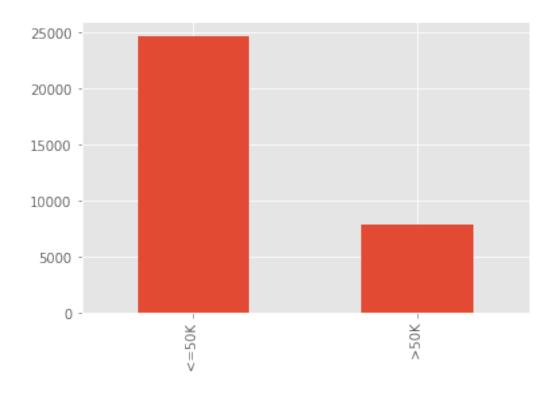
```
[13]: pd.DataFrame.hist(df, figsize = [15,15]);
```



Show a bar graph with the value counts of the attribute high-income. Use the method value\_counts of Pandas, then plot with the option kind = 'bar'

```
[15]: df['high-income'].value_counts().plot(kind = 'bar')
```

[15]: <matplotlib.axes.\_subplots.AxesSubplot at 0x228c9a0f5c0>



### 1.1.1 More examples of figures

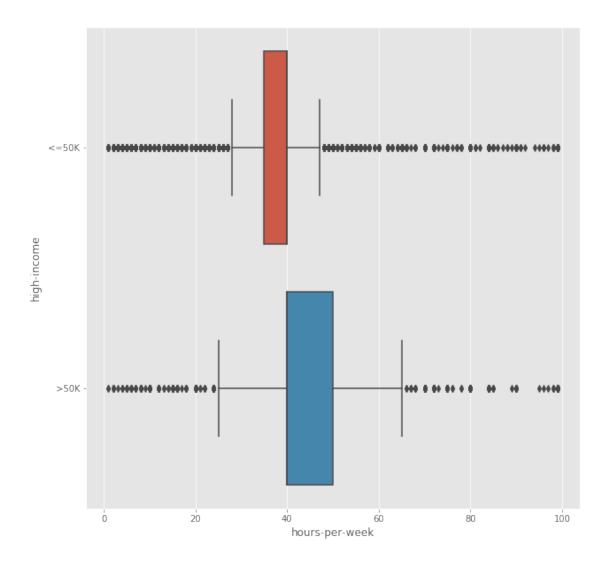
### Boxplot

### More on boxplots

Use the boxplot method of Seaborn with hours-per-week in the x axis and high-income in the y axis. The columns are extracted with the loc method of Pandas DataFrames, with index expression [:,'attribute-name'] (means all the elements of column attribute-name)

```
[16]: plt.figure(figsize = [10,10])
sns.boxplot(x=df.loc[:,'hours-per-week'], y=df.loc[:,'high-income'])
```

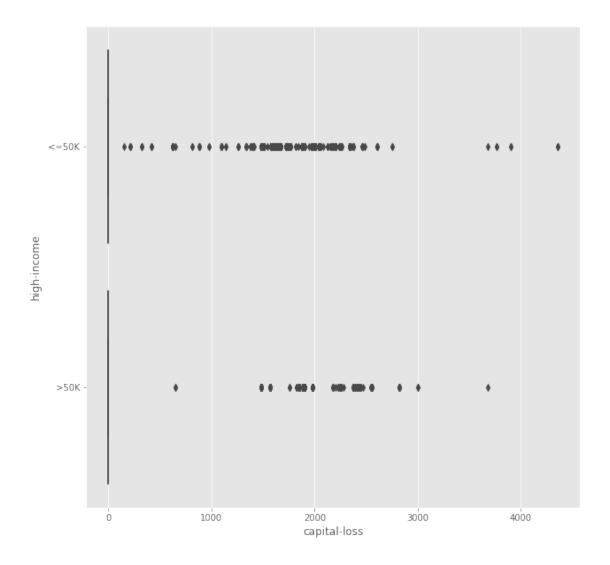
[16]: <matplotlib.axes.\_subplots.AxesSubplot at 0x228c99a1240>



Similar boxplot for 'capital-loss' and 'high-income']

```
[17]: plt.figure(figsize = [10,10])
sns.boxplot(x=df.loc[:,'capital-loss'], y=df.loc[:,'high-income'])
```

[17]: <matplotlib.axes.\_subplots.AxesSubplot at 0x228c99576a0>



Something is wrong, the figure does not look like a proper boxplot.

Let's look at the capital-loss column with the describe method

Name: capital-loss, dtype: float64

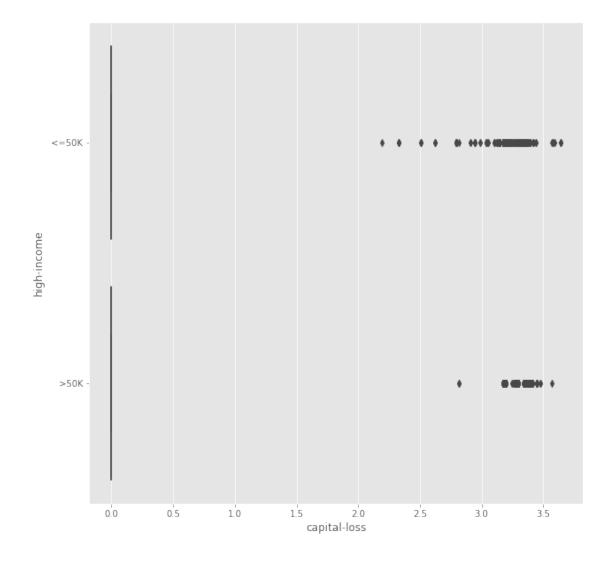
#### [18]: df['capital-loss'].describe() [18]: count 32561.000000 mean 87.303830 402.960219 std 0.000000 min 25% 0.000000 50% 0.000000 75% 0.000000 max 4356.000000

The three quartiles are all zero, and there are no left outliers.

Let's try with a logarithmic transformation (add +1 to deal with the zero values) - use the log10 function of numpy to transform the capital-loss+1 - prepare a plot figure of size [10,10] - boxplot with Seaborn

```
[19]: from numpy import log10
   plt.figure(figsize = [10,10])
   sns.boxplot(x=log10(df.loc[:,'capital-loss']+1), y=df.loc[:,'high-income'])
```

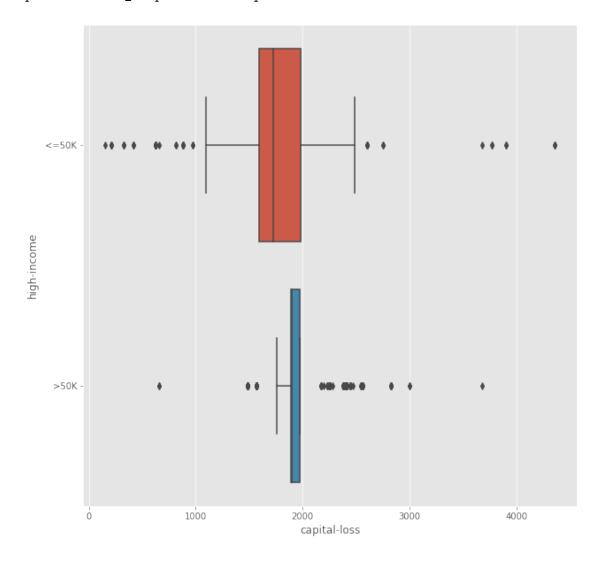
[19]: <matplotlib.axes.\_subplots.AxesSubplot at 0x228c98b95c0>



You can observe that a most of the data are 'compressed' at 0 - it is due to the zero values to which we added 1, whose log is 0 again

Look at the rows with non-zero values: in the x values, instead of the : indicating 'all the rows' we must use a 'selector expression', in this case df['capital-loss']!=0

[20]: <matplotlib.axes.\_subplots.AxesSubplot at 0x228ca1afc50>



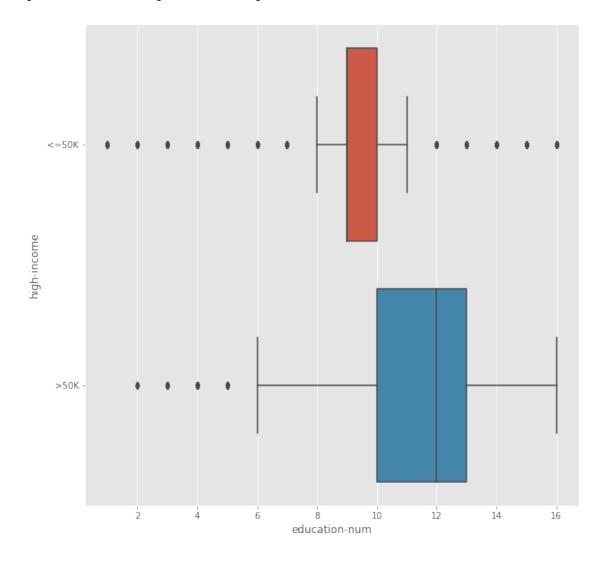
Now we see that the non-zero values have some structure

### 1.1.2 Plot another pair of columns

education-num and high-income

```
[21]: plt.figure(figsize = [10,10])
sns.boxplot(x=df.loc[:,'education-num'], y=df.loc[:,'high-income'])
```

[21]: <matplotlib.axes.\_subplots.AxesSubplot at 0x228c9ac1240>



# dataMining02-data exploration-iris

February 12, 2020

## 1 From UCI Machine Learning Repository

#### 1.1 Iris Dataset

This data file does not have a header with column names.

- Look at the ".names" text file in the Data Folder, read (visually) the column names and store them in a list
- the url is https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.data
- read the file with read\_csv using also the names parameter
- show the head of the file, just for a quick inspection

Notice: Iris is also available directly with the datasets package, together with some other toy datasets used as examples

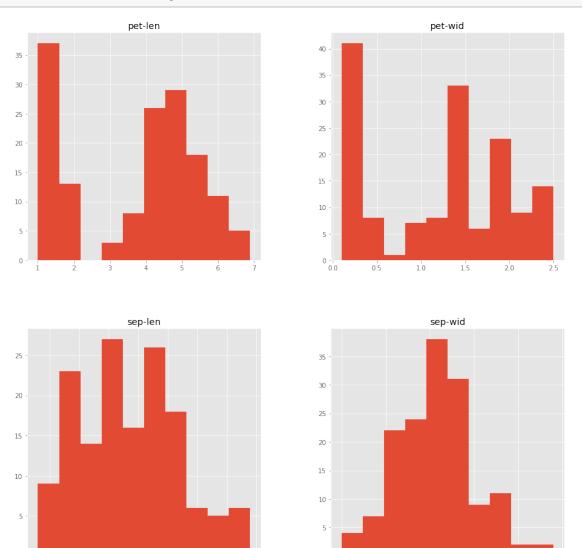
```
[9]: names = ['sep-len', 'sep-wid', 'pet-len', 'pet-wid', 'class']
url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.data'
df = pd.read_csv(url, sep = ',', names = names)
df.head()
```

```
[9]:
                 sep-wid pet-len pet-wid
        sep-len
                                                    class
            5.1
                      3.5
     0
                               1.4
                                        0.2
                                             Iris-setosa
     1
            4.9
                      3.0
                               1.4
                                        0.2 Iris-setosa
            4.7
                      3.2
     2
                               1.3
                                        0.2 Iris-setosa
     3
            4.6
                      3.1
                               1.5
                                        0.2 Iris-setosa
            5.0
                      3.6
                               1.4
                                        0.2 Iris-setosa
```

# 2 Print histogram of numeric values

Use the hist method again

[10]: pd.DataFrame.hist(df, figsize = [15,15]);



### 2.0.1 Print histogram of frequencies for the class value

5.0

6.0

6.5

7.0

7.5

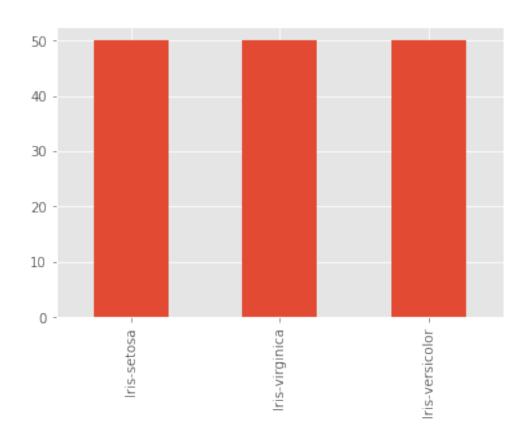
Use the value\_count method on class column, then plot the result with kind = 'bar'

[11]: <matplotlib.axes.\_subplots.AxesSubplot at 0x228c9c15da0>

2.5

3.0

3.5



# dataMining02-data\_exploration-wines

February 12, 2020

## 1 From UCI Machine Learning Repository

### 1.1 Wine Quality Dataset

#### 1.1.1 Read data from archive.

In this case, it is a csv with header In this case, it is a csv with header, separator is ';' The download url is http://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv

Use the read\_csv() method of pandas dataframe https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.read\_csv.html

Use df as the dataframe name

In this dataset the column names are already included in the .csv file

#### 1.1.2 Show column names

Use the columns attribute of pandas on df

## 1.1.3 Show portion of data

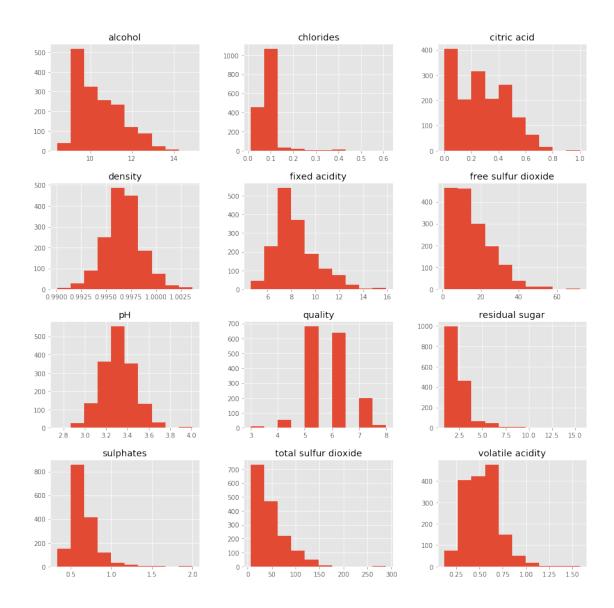
Use the head method of pandas dataframe

4]: df	.head()												
1]:	fixed ac	idity	volat	ile ac	idity	citric	acid	l resid	lual s	ugar	chlori	des	\
0		7.4			0.70		0.00	)		1.9	0.	076	
1		7.8			0.88		0.00	)		2.6	0.	098	
2		7.8			0.76		0.04	<u>l</u>		2.3	0.	092	
3		11.2			0.28		0.56	3		1.9	0.	075	
4		7.4			0.70		0.00	)		1.9	0.	076	
	free sul	fur di	oxide	total	sulfur	dioxid	e d	density	рН	sul	phates	\	
0			11.0			34.	0	0.9978	3.51		0.56		
1			25.0			67.	0	0.9968	3.20	)	0.68		
2			15.0			54.	0	0.9970	3.26	;	0.65		
3			17.0			60.	0	0.9980	3.16	;	0.58		
4			11.0			34.	0	0.9978	3.51		0.56		
	alcohol	quali	ty										
0	9.4		5										
1	9.8		5										
2	9.8		5										
3	9.8		6										
4	9.4		5										

### 1.1.4 Show histograms for all numeric values

Use the DataFrame.hist method of Pandas. You can set the figsize parameter to adjust size

```
[5]: pd.DataFrame.hist(df, figsize = [15,15]);
```



## 1.1.5 Show synthetic description

Use the describe method of Pandas

## [6]: df.describe()

[6]:	fixed acidity	volatile acidity	citric acid	residual sugar
count	1599.000000	1599.000000	1599.000000	1599.000000
mean	8.319637	0.527821	0.270976	2.538806
std	1.741096	0.179060	0.194801	1.409928
min	4.600000	0.120000	0.000000	0.900000
25%	7.100000	0.390000	0.090000	1.900000
50%	7.900000	0.520000	0.260000	2.200000

75% max	9.20000 15.90000		0.640000 0.4 1.580000 1.0			00000 500000	
	2010000				2010		
	chlorides	free sulfur	dioxide to	tal sulf	ur dioxide	density	\
count	1599.000000	1599	.000000	1	599.000000	1599.000000	
mean	0.087467	15	.874922		46.467792	0.996747	
std	0.047065	10	.460157		32.895324	0.001887	
min	0.012000	1	.000000		6.000000	0.990070	
25%	0.070000	7	.000000		22.000000	0.995600	
50%	0.079000	14	.000000		38.000000	0.996750	
75%	0.090000	21	.000000		62.000000	0.997835	
max	0.611000	72	.000000		289.000000	1.003690	
	pН	sulphates	alcoho	l q	uality		
count	1599.000000	1599.000000	1599.00000	0 1599.	000000		
mean	3.311113	0.658149	10.42298	5.	636023		
std	0.154386	0.169507	1.06566	8 0.	807569		
min	2.740000	0.330000	8.40000	0 3.	000000		
25%	3.210000	0.550000	9.50000	0 5.	000000		
50%	3.310000	0.620000	10.20000	0 6.	000000		
75%	3.400000	0.730000	11.10000	0 6.	000000		
max	4.010000	2.000000	14.90000	0 8.	000000		

**Quality** is the target class in this dataset. The **describe** method of pandas dataframes gives a short summary

```
[7]: df['quality'].describe()
```

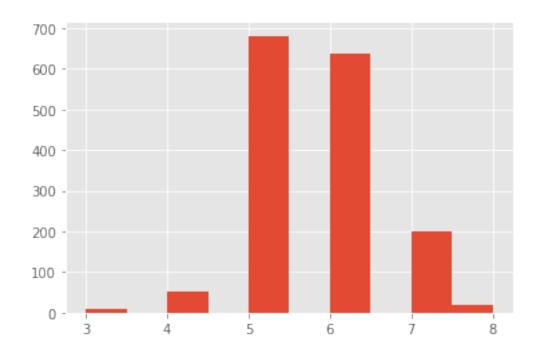
```
1599.000000
[7]: count
     mean
                  5.636023
                  0.807569
     std
     min
                  3.000000
     25%
                  5.000000
     50%
                  6.000000
     75%
                  6.000000
                  8.000000
     max
```

Name: quality, dtype: float64

## 1.1.6 Plot an histogram for "quality"

Use the hist method of matplotlib.pyplot applied to the quality column of df

```
[8]: plt.hist(df['quality'])
plt.show()
```



# ml 03-01-intro-iris

February 12, 2020

This notebook contains an excerpt from the Python Data Science Handbook by Jake VanderPlas; the content is available on GitHub.

The text is released under the CC-BY-NC-ND license, and code is released under the MIT license. If you find this content useful, please consider supporting the work by buying the book!

Adapded for class presentation by Claudio Sartori - University of Bologna

## 1 Introducing Scikit-Learn

Scikit-Learn - package that provides efficient versions of a large number of common algorithms - clean, uniform, and streamlined API - very useful and complete online documentation. - once you understand the basic use and syntax of Scikit-Learn for one type of model, switching to a new model or algorithm is very straightforward

#### 1.1 Contents

- Introduction to Scikit-Learn
- Data representation in Scikit-Learn
- Estimator API
- Examples

#### 1.2 Data Representation in Scikit-Learn

### 1.2.1 Data as table

- a two-dimensional grid of data
  - rows represent individual elements of the dataset
  - columns represent quantities related to each of these elements
- Example: Iris dataset
  - analyzed by Ronald Fisher in 1936
  - download this dataset in the form of a Pandas DataFrame using the seaborn library

```
[1]: import seaborn as sns import pandas as pd
```

Download the Iris dataset at the url https://archive.ics.uci.edu/ml/machine-learning-databases/iris/ir or from your local file, if you already have it. The file does not have header, use as column names the list below, inspect the text file to see which character is used as separator.

'sepal length', 'sepal width', 'petal length', 'petal width', 'species'

Use the dataframe name iris. Show the head of iris

--> Insert your code in new cell below

```
[2]: iris_url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.

data'
iris = pd.read_csv(iris_url, sep = ',', header = None\
, names = ['sepal length', 'sepal width', 'petal length',

→'petal width', 'species'])
iris.head(4) # show first 4 data rows
```

```
[2]:
        sepal length sepal width petal length petal width
                                                                   species
     0
                 5.1
                              3.5
                                             1.4
                                                          0.2 Iris-setosa
                 4.9
                              3.0
                                             1.4
     1
                                                          0.2 Iris-setosa
     2
                 4.7
                              3.2
                                             1.3
                                                          0.2 Iris-setosa
     3
                 4.6
                                            1.5
                                                          0.2 Iris-setosa
                              3.1
```

- each row refers to a single observed flower
  - the number of rows is the total number of flowers in the dataset.
  - sample: a single row
  - n\_samples: number of rows
- each column refers to a piece of information that describes each sample
  - feature: a single column n\_features: the number of columns
    - \* each column has a data type: number (continuous), boolean, discrete (nominal or ordinal, represented with integers or strings)

Features matrix The part of the data matrix containing the unsupervised attributes

Usually in *scikit-learn* documentation referred as X

Can be a: - two-dimensional numpy array with shape [n\_samples, n\_features] - SciPy sparse matrix - Pandas DataFrame

The matrix cases require uniform data types in columns

**Target array** label or target array, by convention usually called y - usually one dimensional, with length n\_samples, - generally contained in a NumPy array or Pandas Series. - may have continuous numerical values, or discrete classes/labels - usually it the quantity we want to predict from the data - in statistical terms, it is the dependent variable

In the example we may wish to construct a model that can predict the species of flower based on the other measurements

The measurements of the flower components are the features array

The species column can be considered the target array

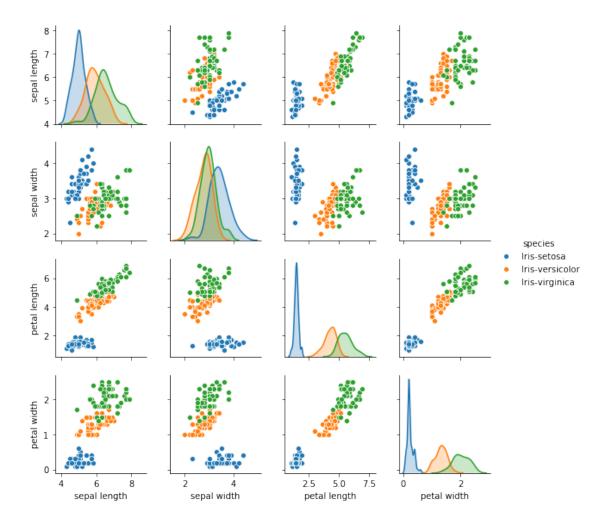
#### 1.2.2 Visualization

Use Seaborn (see Visualization With Seaborn) to visualize the data

Below we need to prepare the environment for plotting information on the dataset.

- 1. issue the command %matplotlib inline In this way, the output of plotting commands is displayed inline within frontends like the Jupyter notebook, directly below the code cell that produced it. The resulting plots will then also be stored in the notebook document.
- 2. import seaborn giving it the 'nickname' sns
- 3. call the pairplot function of seaborn on the iris dataset, with parameters
  - hue = 'species', this sets the meaning of the color in the plot of the points of the dataset
  - height = 2, this sets the size of the plots
- --> insert your code in a new cell below this one

```
[3]: %matplotlib inline
import seaborn as sns
sns.pairplot(iris, hue='species', height=2);
```



For use in Scikit-Learn, we will extract the features matrix and target array from the DataFrame. We can do this using some of the Pandas DataFrame operations discussed in the Chapter 3 of the above mentioned book.

For example, the .drop method allows to drop a column or row by name; remember to specify the axis to use, which is 1 for columns.

### 1.2.3 Preparing features and target

Store in X the content of iris excluding the column species. Verify the shape

--> insert your code in a new cell below this one

```
[4]: X = iris.drop('species', axis=1)
X.shape
```

[4]: (150, 4)

Store in y the column species of iris. Verify the shape

--> insert your code in a new cell below this one

```
[5]: y = iris['species']
y.shape
```

[5]: (150,)

#### 1.3 Scikit-Learn's Estimator API

The Scikit-Learn API is designed with the following guiding principles in mind, as outlined in the Scikit-Learn API paper:

- Consistency: All objects share a common interface drawn from a limited set of methods, with consistent documentation.
- Inspection: All specified parameter values are exposed as public attributes.
- Limited object hierarchy: Only algorithms are represented by Python classes; datasets are represented in standard formats (NumPy arrays, Pandas DataFrames, SciPy sparse matrices) and parameter names use standard Python strings.
- Composition: Many machine learning tasks can be expressed as sequences of more fundamental algorithms, and Scikit-Learn makes use of this wherever possible.
- Sensible defaults: When models require user-specified parameters, the library defines an appropriate default value.

In practice, these principles make Scikit-Learn very easy to use, once the basic principles are understood. Every machine learning algorithm in Scikit-Learn is implemented via the Estimator API, which provides a consistent interface for a wide range of machine learning applications.

#### 1.4 Hyperparameters

The machine learning algorithms are designed to learn from the data the *parameters* that will be used at run time by the algorithms implementing the tasks to perform at the best on data similar to those used in learning.

For example, a decision tree (and in particular all the tests placed in the nodes) are the parameters of a decision tree classifier

The learning process is also controlled by other parameters (e.g. to control the *overfitting* ) which cannot be directly learned from the data, but are chosen *before* the learning process. Those are called **hyperparameters** 

#### 1.4.1 Basics of the API

Most commonly, the steps in using the Scikit-Learn estimator API are as follows (we will step through a handful of detailed examples in the sections that follow).

- 1. Choose a class of model by importing the appropriate estimator class from Scikit-Learn.
- 2. Choose model hyperparameters by instantiating this class with desired values.
  - or in the first attempt use the default values
- 3. Arrange data into a features matrix and target vector following the discussion above.
- 4. Fit the model to your data by calling the fit() method of the model instance.
- 5. Apply the Model to new data:
- For supervised learning, often we predict labels for unknown data using the predict() method.
- For unsupervised learning, we often transform or infer properties of the data using the transform() or predict() method.

We will now step through several simple examples of applying supervised and unsupervised learning methods.

#### 1.4.2 Supervised learning example: Iris classification

Let's take a look at another example of this process, using the Iris dataset we discussed earlier. Our question will be this: given a model trained on a portion of the Iris data, how well can we predict the remaining labels?

For this task, we will use the *Decision Tree* algorithm, with the standard parameter values. We would like to evaluate the model on data it has not seen before, and so we will split the data into a *training set* and a *testing set*. This could be done by hand, but it is more convenient to use the train\_test\_split utility function

- 1. Import the method train\_test\_split from sklearn.model\_selection
- 2. Generate the variables Xtrain, Xtest, ytrain, ytest by calling the function train\_test\_split with parameters X and y, and the additional parameter random\_state = 1
- 3. Show the shape of the resulting variables
- --> insert your code in a new cell below this one

```
[6]: from sklearn.model_selection import train_test_split
Xtrain, Xtest, ytrain, ytest = train_test_split(X, y, random_state=1)
print(Xtrain.shape, Xtest.shape, ytrain.shape, ytest.shape)
```

```
(112, 4) (38, 4) (112,) (38,)
```

With the data arranged, we can follow our recipe to predict the labels: 1. choose the model class, it will be DecisionTreeClassifier, imported from sklearn.tree 2. instantiate the model as a DecisionTreeClassifier whithout any hyperparameter, we will use the defaults 3. fit the model to data, calling its method fit with parameters Xtrain, ytrain 4. predict the target ytrain\_model using the predict method of model on the Xtrain data

--> insert your code in a new cell below this one

```
[7]: from sklearn.tree import DecisionTreeClassifier # 1. choose model class model = DecisionTreeClassifier(criterion = 'entropy') # 2. instantiate model model.fit(Xtrain, ytrain) # 3. fit model to data
```

```
ytrain_model = model.predict(Xtrain) # 4. fir model to⊔

→ training data
```

We can use the accuracy\_score utility to see the fraction of predicted training set labels that match their true value.

Import the accuracy\_score from sklearn.metrics and call it on ytrain, ytrain\_model

--> insert your code in a new cell below this one

```
[8]: from sklearn.metrics import accuracy_score
accuracy_train = accuracy_score(ytrain, ytrain_model)
print("The accuracy on training set is {0:.2f}%".format(accuracy_train * 100))
```

The accuracy on training set is 100.00%

Finally, predict the new target ytest\_model using the predict method of model on the Xtest data, then compute the accuracy on the test set

--> insert your code in a new cell below this one

```
[9]: ytest_model = model.predict(Xtest) # 4. predict on new data
accuracy_test = accuracy_score(ytest, ytest_model)
print("The accuracy on test set is {0:.2f}%".format(accuracy_test * 100))
```

The accuracy on test set is 97.37%

#### 1.5 Show the Decision Tree

To show the Decision Tree we will need a few imports

```
from matplotlib import pyplot from sklearn.tree import plot_tre from matplotlib.pyplot import figure
```

We will start setting the *figure size* with the **figure** function, taking as argument **figsize** and a list of two values in inches, try and error for the measures you like.

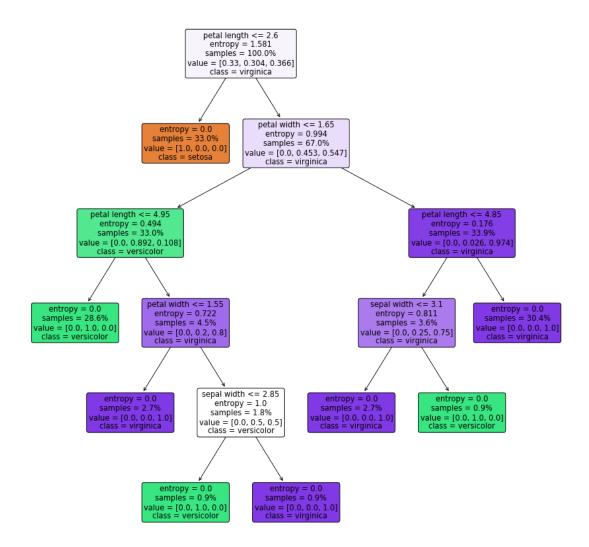
We will then use the plot\_tree function of sklearn.tree. It takes as argument the *fitted model*, in our case model and several arguments to control how the tree is displayed.

I suggest the arguments below, you can try freely configurations and omissions of the parameters, to use the defaults. The parameters must follow the model variable and be separated by commas, the order is not relevant, since the parameters are named.

filled=True feature\_names = ['sepal length', 'sepal width' , 'petal length', 'petal width'] <br/>
width'] <br/>
s\_names = ['setosa', 'versicolor', 'virginica'] <br/>
frames = True <br/>
proportion = True <br/>
proportion = True <br/>
frames = ['setosa', 'versicolor', 'virginica'] <br/>
frames = True <br/>
frames = ['setosa', 'versicolor', 'virginica'] <br/>
frames = True <br/>
frames = ['setosa', 'versicolor', 'virginica'] <br/>
frames = True <br/>
frames = ['setosa', 'versicolor', 'virginica'] <br/>
frames = ['setosa', 'versicolor', 'virginica'] <br/>
frames = True <br/>
frames

--> insert your code in a new cell below this one

```
[10]: from matplotlib import pyplot from sklearn.tree import plot_tree
```



# ml-03-02a-pruning\_example

February 12, 2020

## 1 Pruning the Decision Tree

In this example we are directly given two different datasets, one will be used for training, the other for testing.

We will start training the model with the training data, then testing it with the test data.

Then we will observe the resulting tree, and try to improve the result with pruning.

Start importing pandas and numpy, then assign to the variables in\_train and in\_test the strings binaries\_train.csv and binaries\_test.csv.

--> Insert your code in a new cell after this one

```
[1]: import pandas as pd
import numpy as np
in_train = 'binaries_train.csv'
in_test = 'binaries_test.csv'
```

Read the in\_train file into the train dataframe and inspect it.

--> Insert your code in a new cell after this one

```
[2]: train = pd.read_csv(in_train)
train.head()
```

```
[2]:
         B1
              B2
                   В3
                         B4
                              В5
                                   B6
                                       Class
                     0
                0
      1
           0
                     0
                          0
                               0
                                    1
                                             1
      2
           0
                0
                     0
                          0
                               1
                                    0
                                             0
                0
                                             1
      3
           0
                     0
                          0
                               1
                                    1
           0
                0
                     0
                          1
                               0
                                    0
                                             1
```

Prepare the X\_train variable, by dropping the last column of train, and the y\_train variable with the last column of train, then inspect the shapes.

```
[3]: X_train = train.drop(train.columns[-1], axis = 1) # drop the last column X_train.shape
```

```
[3]: (64, 6)
```

```
[4]: #y_train = train.drop(train.columns[0:-1], axis = 1) # drop all the columns but

→ the last

y_train = train.iloc[:,-1]

y_train.shape
```

[4]: (64,)

#### 1.1 Train a full tree

With the fit method we will train the **Decision Tree**.

The parameters for the training are set in the creation of the model.

In this case we will set only the 'split criterion' to entropy. Don't forget to import the tree.DecisionTreeClassifier from sklearn.

--> Insert your code in a new cell after this one

```
[5]: from sklearn import tree
  model = tree.DecisionTreeClassifier(criterion="entropy")
  model.fit(X_train, y_train)
```

```
[5]: DecisionTreeClassifier(class_weight=None, criterion='entropy', max_depth=None, max_features=None, max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, min_samples_leaf=1, min_samples_split=2, min_weight_fraction_leaf=0.0, presort=False, random state=None, splitter='best')
```

Now use the trained model to predict y\_predicted\_train from X\_train.

Evaluate the percentage of matches between y\_predicted\_train and y\_train.

Hint: you can use np.mean on the comparison of the two vectors.

--> Insert your code in a new cell after this one

```
[6]: y_predicted_train = model.predict(X_train)
```

```
[7]: accuracy_train = np.mean(y_train == y_predicted_train) * 100
print("The accuracy on training set is {0:.1f}%".format(accuracy_train))
```

The accuracy on training set is 100.0%

Now we load the test set, make the prediction using the already trained model and compute the accuracy.

```
[8]: test=pd.read_csv(in_test)
X_test = test.drop(test.columns[-1], axis = 1) # drop the last column
y_test = test.iloc[:,-1] # keep only the last column
y_predicted_test = model.predict(X_test)
accuracy_test = np.mean(y_test == y_predicted_test) * 100
print("The accuracy on test set is {0:.1f}%".format(accuracy_test))
```

The accuracy on test set is 60.9%

#### 1.1.1 Observe the tree

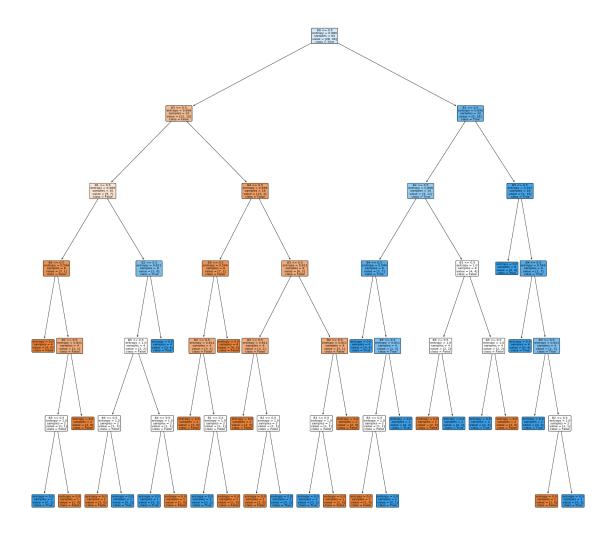
Import the following and set the size of the figure as below

```
from matplotlib.pyplot import figure figure(figsize = (25,25))
```

Plot the tree with the tree.plot\_tree function. Use as parameters the model, rounded = True, filled = True.

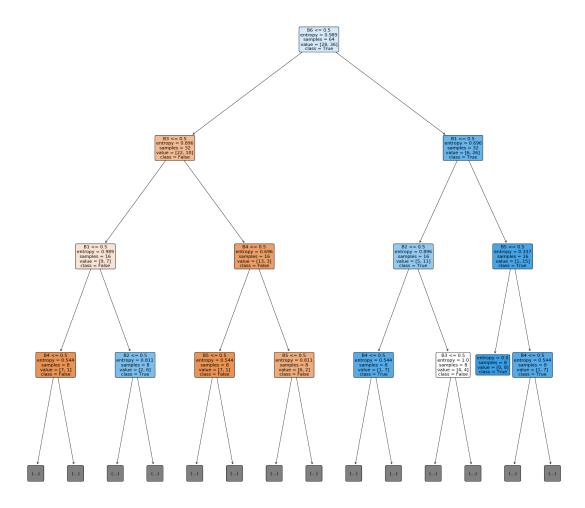
Use as feature\_names the column names of train. Use as class\_names 'False' and 'True'

The tree generated has a number of internal node levels equal to the number of predicting attributes.



Try to understand better the tree by plotting only the first two levels under the root. This is obtained with the parameter max\_depth = 3. Remember that here we are not changing the tree, but only displaying the upper part of the tree.

```
figure(figsize = (25,25))
tree.plot_tree(model
    , filled=True
    , feature_names = train.columns
    , class_names = ['False', 'True']
    , rounded = True
    , max_depth = 3
    );
```



#### 1.2 Pruned tree

From the observation of the tree, choose an appropriate value for max\_dept and redo the training using the parameter max\_depth = max\_depth in the fit method. Compute the accuracy on the training set, and then on the test set.

```
[11]: max_depth = 1
model_pruned = tree.DecisionTreeClassifier(criterion="entropy", max_depth = 
    →max_depth)
model_pruned.fit(X_train, y_train)
y_predicted_train_pruned = model_pruned.predict(X_train)
```

The accuracy of the pruned tree on training set is 75.0%

The accuracy of the pruned tree on test set is 76.6%

# ml-03-02b-class-w-hyperp-tuning

February 12, 2020

©Claudio Sartori - Module: Machine Learning - Classification

## 1 Classification with hyperparameter tuning

#### 1.0.1 aim:

Show classification with different strategies for the tuning and evaluation of the classifier 1. simple holdout 2. holdout with validation train and validate repeatedly changing a hyperparameter, to find the value giving the best score, then test for the final score 3. cross validation on training set, then score on test set 4. bagging it is an *ensemble* method made available in scikit-learn

**NB**: You should not interpret those experiments as a way to find the *best* evaluation method, but simply as examples of *how* to do the evaluation.

If you look at the final report, methods 1 to 3 are meant for increasing evaluation reliability, method 3 is the more reliable, but it requires several repetitions for cross validation, therefore, if the learning method is expensive, it requires long processing time. If, due to intrinsic variation caused by random sampling, it turns out that methods 1 or 2 give higher accuracy, this means simply that the forecast towards generalisation is less reliable.

Method 4 is on a different dimension, it simply shows that a good result can be obtained with an *ensemble* of simpler classifiers (the best value for the hyperparameter max\_depth is smaller than in the other cases)

#### 1.0.2 Workflow

- download the data
- drop the useless data
- separe the predicting attributes X from the class attribute y
- split X and y into training and test
- part 1 single run with default parameters
  - initialise an estimator with the chosen model generator
  - fit the estimator with the training part of X
  - show the tree structure
  - part 1.1
    - \* predict the y values with the fitted estimator and the train data

- · compare the predicted values with the true ones and compute the accuracy on the training set
- part 1.2
  - \* predict the y values with the fitted estimator and the test data
    - · compare the predicted values with the true ones and compute the accuracy on the test set
- part 2 multiple runs changing a parameter
  - prepare the structure to hold the accuracy data for the multiple runs
  - repeat for all the values of the parameter
    - \* initialise an estimator with the current parameter value
    - \* fit the estimator with the training part
    - \* predict the class for the test part
    - \* compute the accuracy and store the value
  - find the parameter value for the top accuracy
- part 3 compute accuracy with cross validation
  - prepare the structure to hold the accuracy data for the multiple runs
  - repeat for all the values of the parameter
    - \* initialise an estimator with the current parameter value
    - \* compute the accuracy with cross validation and store the value
  - find the parameter value for the top accuracy
  - fit the estimator with the entire X
  - show the resulting tree and classification report

The data are already in your folder, use the name winequality-red.csv

```
[1]: import pandas as pd
    import numpy as np
    import matplotlib.pyplot as plt
    from sklearn import tree
    from sklearn.metrics import accuracy_score, classification_report,_
     from sklearn.model selection import cross val score
    from sklearn.ensemble import BaggingClassifier
    %matplotlib inline
    plt.rcParams['figure.figsize'] = [20, 20]
    random state = 15
    np.random.seed(random_state)
    # the random state is reset here in numpy, all the scikit-learn procedure use,
     → the numpy random state
     # obviously the experiment can be repeated exactly only with a complete run of |
     → the program
     #data_url = "uci_breast_tissue_data/BreastTissue.csv"
    data_url = "winequality-red.csv"
    target_name = 'quality'
    to_drop = []
```

```
# parameter_values to be determined after the fitting of the full tree
df = pd.read_csv(data_url , sep = ';')
print("Shape of the input data {}".format(df.shape))
```

Shape of the input data (1599, 12)

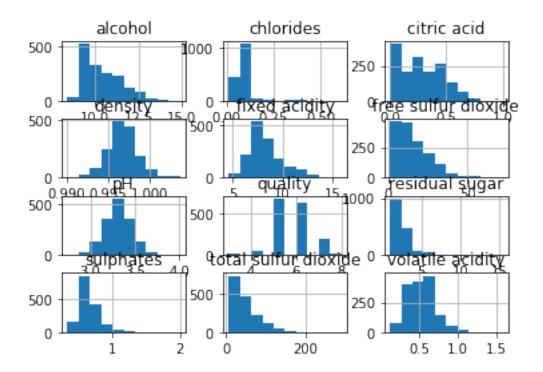
Have a quick look to the data. - use the .shape attribute to see the size - use the .head() function to see column names and some data - use the .hist() method for an histogram of the columns - use the .unique method to see the class values

```
[2]: df.head()
[2]:
        fixed acidity
                       volatile acidity citric acid residual sugar
                                                                           chlorides
                                                   0.00
                   7.4
                                     0.70
                                                                     1.9
                                                                               0.076
     1
                   7.8
                                     0.88
                                                   0.00
                                                                     2.6
                                                                               0.098
     2
                   7.8
                                     0.76
                                                   0.04
                                                                     2.3
                                                                               0.092
     3
                  11.2
                                     0.28
                                                   0.56
                                                                     1.9
                                                                               0.075
     4
                   7.4
                                     0.70
                                                   0.00
                                                                     1.9
                                                                               0.076
        free sulfur dioxide
                              total sulfur dioxide density
                                                                     sulphates
                                                                  рΗ
                        11.0
                                                34.0
                                                       0.9978
                                                                            0.56
     0
                                                                3.51
                                                67.0
     1
                        25.0
                                                       0.9968
                                                                3.20
                                                                            0.68
     2
                        15.0
                                                54.0
                                                       0.9970
                                                                3.26
                                                                            0.65
     3
                        17.0
                                                60.0
                                                       0.9980
                                                                            0.58
                                                                3.16
     4
                        11.0
                                                34.0
                                                       0.9978 3.51
                                                                            0.56
        alcohol
                 quality
            9.4
     0
                        5
            9.8
                        5
     1
                        5
     2
            9.8
     3
            9.8
                        6
     4
            9.4
                        5
```

Use the hist method of the DataFrame to show the histograms of the attributes

NB: a semicolon at the end of a statement suppresses the Out[]

```
[3]: df.hist();
```



Print the unique class labels (hint: use the unique method of pandas Series

```
[4]: classes = df[target_name].unique()
    classes.sort()
    print(classes)
```

[3 4 5 6 7 8]

Split the data into the predicting values X and the class y Drop also the columns which are not relevant for training a classifier, if any

The method "drop" of dataframes allows to drop either rows or columns - the "axis" parameter chooses between dropping rows (axis=0) or columns (axis=1)

```
[5]: X = df.drop([target_name], axis = 1) # drop the class column
y = df[target_name] # Class only
```

Another quick look to data

# [6]: X.head()

[6]:	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	\
0	7.4	0.70	0.00	1.9	0.076	
1	7.8	0.88	0.00	2.6	0.098	
2	7.8	0.76	0.04	2.3	0.092	

```
3
                  11.2
                                     0.28
                                                   0.56
                                                                     1.9
                                                                               0.075
     4
                   7.4
                                     0.70
                                                   0.00
                                                                     1.9
                                                                               0.076
        free sulfur dioxide
                              total sulfur dioxide
                                                      density
                                                                  pH sulphates
     0
                        11.0
                                                       0.9978
                                                                3.51
                                                                           0.56
                        25.0
                                                67.0
                                                       0.9968
                                                                           0.68
     1
                                                                3.20
     2
                        15.0
                                                54.0
                                                       0.9970 3.26
                                                                           0.65
     3
                        17.0
                                                60.0
                                                       0.9980
                                                               3.16
                                                                           0.58
     4
                                                                           0.56
                        11.0
                                                34.0
                                                       0.9978 3.51
        alcohol
     0
            9.4
            9.8
     1
     2
            9.8
     3
            9.8
     4
            9.4
[7]: y.head()
[7]: 0
          5
```

# 1.1 Prepare a simple model selection: holdout method

• Split X and y in train and test

Name: quality, dtype: int64

• Show the number of samples in train and test, show the number of features

There are 1199 samples in the training dataset There are 400 samples in the testing dataset Each sample has 11 features

#### 1.2 Part 1

1

2

3

5

5

6 5

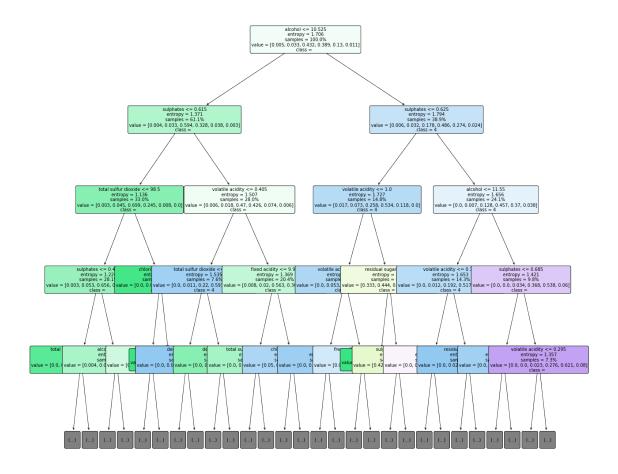
• Initialize an estimator with the required model generator tree.DecisionTreeClassifier(criterion="entropy")

• Fit the estimator on the train data and target

```
[9]: estimator = tree.DecisionTreeClassifier(criterion="entropy")
    estimator.fit(X_train, y_train);
```

Look at the tree structure - the feature names are used to show the tests in the nodes - they are the column names in the X - the class names - the attribute <code>estimator.classes\_</code> contains the array of classes detected in the target; if the classes are numbers they have to be transformed in strings with str() - the dept of the visualization can be limited with the parameter  $max_depth$ 

```
plt.figure(figsize = (20,20)) tree.plot_tree(estimator
     , feature_names = X.columns
                                           , class_names = str(estimator.classes_)
     , rounded = True
                                 , proportion = True
                                                                 , max_depth = 1
     );
[10]: plt.figure(figsize = (20,20),
                  dpi = 500, # this increments the detail, to do a more detiled
       \rightarrow inspection
                )
      tree.plot_tree(estimator
                 , filled=True
                 , feature_names = X.columns
                 , class_names = str(estimator.classes_)
                 , rounded = True
                 , proportion = True
                 , fontsize = 10
                 , max depth = 4 # limited view, since the full tree is very complex
                    );
```



#### 1.2.1 Part 1.1

Let's see how it works on training data - predict the target using the fitted estimator on the training data - compute the accuracy on the training set using accuracy\_score(<target>,,curacy\_score(<target>,

```
[11]: y_predicted_train = estimator.predict(X_train)
accuracy_train = accuracy_score(y_predicted_train, y_train)*100
print("The accuracy on training set is {0:.1f}%".format(accuracy_train))
```

The accuracy on training set is 100.0%

## 1.2.2 Part 1.2

That's more significant: how it works on test data - use the fitted estimator to predict using the test features - compute the accuracy and store it on a variable for the final summary - store the

maximum depth of the tree, for later use - fitted\_max\_depth = estimator.tree\_.max\_depth - store the range of the parameter which will be used for tuning - parameter\_values = range(1,fitted\_max\_depth+1) - print the accuracy on the test set and the maximum depth of the tree

```
[12]: y_predicted_test = estimator.predict(X_test)
    accuracy_ho = accuracy_score(y_test, y_predicted_test) * 100
    fitted_max_depth = estimator.tree_.max_depth
    print("The accuracy on test set is {0:.1f}%".format(accuracy_ho))
    print("The maximum depth of the fitted tree is {}".format(fitted_max_depth))
    parameter_values = range(1,fitted_max_depth+1)
```

The accuracy on test set is 58.8%
The maximum depth of the fitted tree is 16

### 1.3 Part 2

Optimising the tree: limit the maximum tree depth. We will use the three way splitting: train, validation, test. For simplicity, since we already splitted in *train* and *test*, we will furtherly split the *train* - split the training set into two parts: train\_t and val - max\_depth - pruning the tree cutting the branches which exceed max\_depth - the experiment is repeated varying the parameter from 1 to the depth of the unpruned tree - the scores for the various values are collected and plotted

```
[13]: X_train_t, X_val, y_train_t, y_val = train_test_split(X_train , y_train , y_train , random_state = ___ 
→random_state) # default Train 0.75- Test 0.25

print("There are {} samples in the training dataset".format(X_train_t.shape[0]))
print("There are {} samples in the validation dataset".format(X_val.shape[0]))
```

There are 899 samples in the training dataset There are 300 samples in the validation dataset

#### 1.3.1 Loop for computing the score varying the hyperparameter

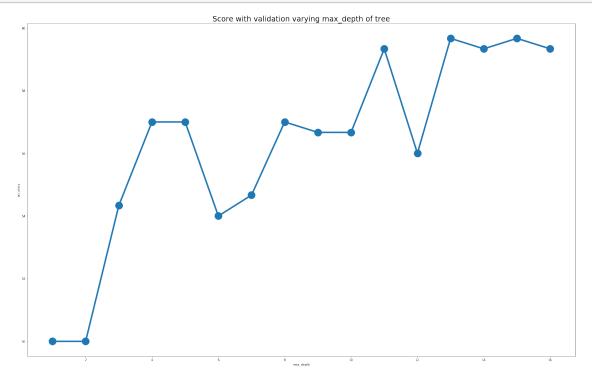
- initialise a list to contain the scores
- loop varying par in parameter\_values
  - initialize an estimator with a DecisionTreeClassifier, using par as maximum depth and entropy as criterion
  - fit the estimator on the train\_t part of the features and the target
  - predict with the estimator using the validation features
  - compute the score comparing the prediction with the validation target and append it to the end of the list

```
[14]: scores = [] # all_scores = []
```

## 1.3.2 Plot the results

Plot using the parameter\_values and the list of scores

```
[15]: plt.figure(figsize=(32,20))
    plt.plot(parameter_values, scores, '-o', linewidth=5, markersize=24)
    plt.xlabel('max_depth')
    plt.ylabel('accuracy')
    plt.title("Score with validation varying max_depth of tree", fontsize = 24)
    plt.show();
```



## 1.3.3 Fit the tree after validation and print summary

- store the parameter value giving the best score with np.argmax(scores)
- initialize an estimator as a DecisionTreeClassifier, using the best parameter value computed above as maximum depth and entropy as criterion
- fit the estimator using the train part
- use the fitted estimator to predict using the test features
- compute the accuracy on the test and store it on a variable for the final summary
- print the accuracy on the test set and the best parameter value

```
[16]: top_par_hov = parameter_values[np.argmax(scores)]
    estimator = tree.DecisionTreeClassifier(criterion="entropy", max_depth = top_par_hov)
    estimator.fit(X_train, y_train)
    y_predicted_test = estimator.predict(X_test)
    accuracy_hov = accuracy_score(y_predicted_test, y_test) * 100
    print("The top accuracy is {0:.1f}%".format(accuracy_hov))
    print("Obtained with max_depth = {}".format(top_par_hov))
```

The top accuracy is 56.0% Obtained with max depth = 13

## 1.4 Part 3 - Tuning with Cross Validation

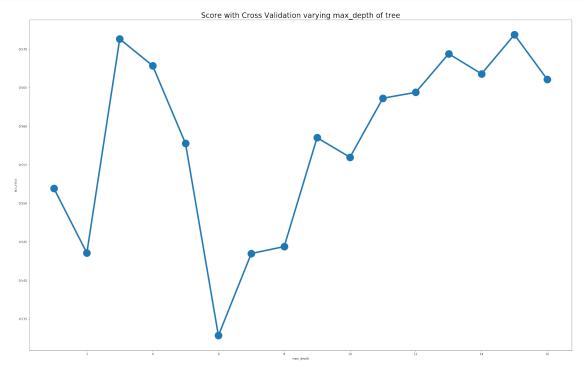
Optimisation of the hyperparameter with **cross validation** (cv suffix in the variable names). Now we will tune the hyperparameter looping on cross validation with the **training set**, then we will fit the estimator on the training set and evaluate the performance on the **test set** 

- initialize an empty list for the scores
- loop varying par in parameter\_values
  - initialize an estimator with a DecisionTreeClassifier, using par as maximum depth and entropy as criterion
  - compute the score using the estimator on the train part of the features and the target using
    - \* cross\_val\_score(estimator, X\_train, y\_train, scoring='accuracy', cv =
      5)
    - \* the result is list of scores
  - compute the average of the scores and append it to the end of the list
- print the scores

```
avg_scores.append(np.mean(scores))
print(avg_scores)
```

```
[0.5519152314979172, 0.5435525832020326, 0.5713089389088722, 0.5678437532607689, 0.5577529689800829, 0.5328357011331578, 0.5434774526459061, 0.5443793438898566, 0.5585019217156184, 0.5559627582243493, 0.5636209817495066, 0.5643876543587679, 0.5693922353804821, 0.5667868463793229, 0.571864056684633, 0.566054670861477]
```

Plot using the parameter\_values and the list of scores



## 1.4.1 Fit the tree after cross validation and print summary

- store the parameter value giving the best score with np.argmax(scores)
- initialize an estimator as a DecisionTreeClassifier, using the best parameter value computed above as maximum depth and entropy as criterion
- fit the estimator using the train part

- use the fitted estimator to predict using the test features
- compute the accuracy on the test and store it on a variable for the final summary
- print the accuracy on the test set and the best parameter value

The accuracy on test set tuned with cross\_validation is 59.2% with depth 15 print(classification\_report(y\_test, y\_predicted))

## [20]: print(classification\_report(y\_test, y\_predicted))

	precision	recall	f1-score	support
3	0.00	0.00	0.00	4
4	0.00	0.00	0.00	14
5	0.65	0.69	0.67	163
6	0.61	0.58	0.59	171
7	0.46	0.58	0.52	43
8	0.25	0.20	0.22	5
accuracy			0.59	400
macro avg	0.33	0.34	0.33	400
weighted avg	0.58	0.59	0.59	400

- micro: Calculate metrics globally by counting the total true positives, false negatives and false positives.
- macro: Calculate metrics for each label, and find their unweighted mean. This does not take label imbalance into account.
- weighted: Calculate metrics for each label, and find their average weighted by support (the number of true instances for each label). This alters 'macro' to account for label imbalance; it can result in an F-score that is not between precision and recall.

print(confusion\_matrix(y\_test, y\_predicted))

## [21]: print(confusion\_matrix(y\_test, y\_predicted))

```
ГΓ
                             0]
    0
         0
              8
                   5
                        1
                             0]
    1
         6 112
                 40
                        4
                             0]
Γ
                 99
                      23
                             3]
```

```
[ 0 0 3 15 25 0]
[ 0 0 0 3 1 1]]
```

## 2 4. Tuning with an ensemble method

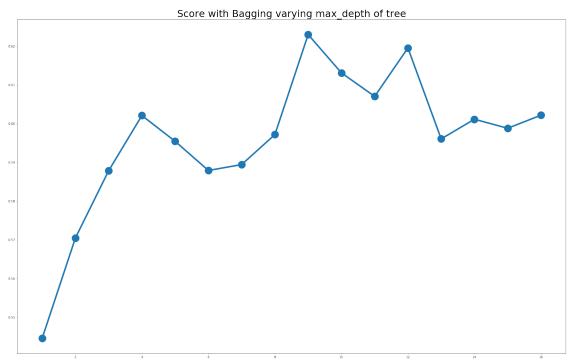
We will use the **bagging** method, made available by **scikit-learn**, for documentation see the pdf file provided, or the online documentation. - initialize an empty list for the scores - loop varying par in parameter\_values - initialize an estimator with a BaggingClassifier applied to a DecisionTreeClassifier, using par as maximum depth and **entropy** as criterion (see below the statement) - fit the estimator on the **train** part - compute an array of cv\_scores using the cross validation method on the estimator on the **train** part of the features and the target, with the accuracy as scoring and 5 folds, then append the mean of the cv\_scores obtained to the end of the list - print the list of scores

```
# use this in the loop for tuning the hyperparameter
                                                                     # estimator_bagging
     = BaggingClassifier(tree.DecisionTreeClassifier(criterion="entropy"
                                                                            , max_depth
                                                                                   )
     = par
     , max_samples=0.5, max_features=0.5 #
[22]: scores_bagging = []
      for par in parameter_values:
          estimator_bagging = BaggingClassifier(tree.
       →DecisionTreeClassifier(criterion="entropy"
                                                   , max_depth = par
                                                 , max_samples=0.5
                                                  max_features=0.5
          estimator bagging.fit(X train, y train)
          scores = cross_val_score(estimator_bagging, X_train, y_train
                                     scoring='accuracy', cv = 5
          scores_bagging.append(np.mean(scores))
      print(scores_bagging)
```

 $\begin{bmatrix} 0.5445619507841822, & 0.570472844903677, & 0.5878375361546816, & 0.6020880744152197, \\ 0.59542980042151, & 0.5879047203227652, & 0.5894282120448173, & 0.5971717597546949, \\ 0.6229901491890222, & 0.613106868693959, & 0.6070268680837339, & 0.6195394112095709, \\ 0.5960569201272726, & 0.6011280851408065, & 0.5988003934025972, & 0.6021653693630428 \end{bmatrix}$ 

Plot the scores, as done in the previous cases

```
, '-o', linewidth=5
, markersize=24
);
```



## 2.0.1 Fit the tree after bagging and print summary

- store the parameter value giving the best score with np.argmax(scores)
- initialize an estimator as above, using the best parameter value computed above as maximum depth and entropy as criterion
- fit the estimator using the train part
- use the fitted estimator to predict using the test features
- compute the accuracy on the test and store it on a variable for the final summary
- print the accuracy on the test set and the best parameter value

```
[24]: top_par_bagging = parameter_values[np.argmax(scores_bagging)]
estimator_bagging = BaggingClassifier(tree.

→DecisionTreeClassifier(criterion="entropy"

, max_depth = top_par_bagging
)

, max_samples=0.5
, max_features=0.5
)
```

The accuracy on test set tuned with bagging is 61.5% Obtained with max\_depth = 9

## 2.0.2 Final report

Print a summary of the four experiments

```
[25]: print("
                                                                Hyperparameter")
                                                     Accuracy
      print("Simple HoldOut and full tree
                                                     {:.1f}%
                                                                  {}".

→format(accuracy_ho, fitted_max_depth))
      print("HoldOut and tuning on validation set:
                                                                  {}".
                                                     {:.1f}%
      →format(accuracy_hov, top_par_hov))
      print("CrossValidation and tuning
                                                                  {}".
                                                     {:.1f}%
      →format(accuracy_cv, top_par_cv))
      print("Ensemble Bagging and tuning
                                                     {:.1f}%
                                                                  {}".
       →format(accuracy_bagging, top_par_bagging))
```

Accuracy Hyperparameter Simple HoldOut and full tree : 58.8% 16
HoldOut and tuning on validation set: 56.0% 13
CrossValidation and tuning : 59.2% 15
Ensemble Bagging and tuning : 61.5% 9

```
[26]: import sklearn print('The scikit-learn version is {}.'.format(sklearn.__version__))
```

The scikit-learn version is 0.21.3.

## 2.0.3 Suggested exercises

- try other datasets
- try to optimise the parameters "min\_impurity\_decrease" "min\_samples\_leaf" and "min\_samples\_split"

# ml-03-03-using-several-classifiers

February 12, 2020

# 1 Using several classifiers and tuning parameters - Parameters grid

#### From official scikit-learn documentation

Adapted by Claudio Sartori

Example of usage of the *model selection* features of scikit-learn and comparison of several classification methods. 1. import a sample dataset 1. split the dataset into two parts: train and test - the *train* part will be used for training and validation (i.e. for *development*) - the *test* part will be used for test (i.e. for *evaluation*) - the fraction of test data will be ts (a value of your choice between 0.2 and 0.5) 1. the function GridSearchCV iterates a cross validation experiment to train and test a model with different combinations of parameter values - for each parameter we set a list of values to test, the function will generate all the combinations - we choose a *score function* which will be used for the optimization - e.g. accuracy\_score, precision\_score, cohen\_kappa\_score, f1\_score, see this page for reference - the output is a dictionary containing - the set of parameters which maximize the score - the test scores 1. prepare the parameters for the grid - it is a list of dictionaries 1. set the parameters by cross validation and the *score functions* to choose from 1. Loop on scores and, for each score, loop on the model labels (see details below)

```
[1]: """
     http://scikit-learn.org/stable/auto_examples/model_selection/
     \hookrightarrow plot\_grid\_search\_digits.html
     Qauthor: scikit-learn.org and Claudio Sartori
     import warnings
     warnings.filterwarnings('ignore') # uncomment this line to suppress warnings
     from sklearn import datasets
     from sklearn.model selection import train test split
     from sklearn.model_selection import GridSearchCV
     from sklearn.metrics import classification_report
     from sklearn.svm import SVC
     from sklearn.linear_model import Perceptron
     from sklearn.neural_network import MLPClassifier
     from sklearn.tree import DecisionTreeClassifier
     from sklearn.naive_bayes import GaussianNB
     from sklearn.neighbors import KNeighborsClassifier
```

```
http://scikit-
```

learn.org/stable/auto\_examples/model\_selection/plot\_grid\_search\_digits.html
@author: scikit-learn.org and Claudio Sartori

## 1.0.1 Prepare the environment

The dataset module contains, among others, a few sample datasets.

See this page for reference

Prepare the data and the target in X and y. Set ts. Set the random state

```
[2]: X = dataset.data
y = dataset.target
ts = 0.3
random_state = 42
```

Split the dataset into the train and test parts

```
[3]: X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=ts, random_state=random_state)
print("Training on %d examples" % len(X_train))
```

Training on 105 examples

The code below is intended to ease the remainder of the exercise

```
tuned_param_dt = [{'max_depth': [range(1,20)]}]
tuned_param_nb = [{'var_smoothing': [10, 1, 1e-1, 1e-2, 1e-3, 1e-4, 1e-5, 1e-6,__
\rightarrow1e-07, 1e-8, 1e-9, 1e-10]}]
tuned_param_lp = [{'early_stopping': [True]}]
tuned_param_svc = [{'kernel': ['rbf'],
                     'gamma': [1e-3, 1e-4],
                     'C': [1, 10, 100, 1000],
                    },
                    {'kernel': ['linear'],
                     'C': [1, 10, 100, 1000],
                    },
                   1
tuned_param_knn =[{'n_neighbors': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]}]
models = {
    'dt': {'name': 'Decision Tree
           'estimator': DecisionTreeClassifier(),
           'param': tuned_param_dt,
          },
    'nb': {'name': 'Gaussian Naive Bayes',
           'estimator': GaussianNB(),
           'param': tuned_param_nb
          },
    'lp': {'name': 'Linear Perceptron
           'estimator': Perceptron(),
           'param': tuned_param_lp,
          },
    'svc':{'name': 'Support Vector
           'estimator': SVC(),
           'param': tuned_param_svc
          },
    'knn':{'name': 'K Nearest Neighbor ',
           'estimator': KNeighborsClassifier(),
           'param': tuned_param_knn
    }
}
scores = ['precision', 'recall']
```

## 1.0.2 The function below groups all the outputs

Write a function which has as parameter the fitted model and uses the components of the fitted model to inspect the results of the search with the parameters grid.

The components are: model.best\_params\_model.cv\_results\_['mean\_test\_score']model.cv\_results\_['std model.cv\_results\_['params']

The classification report is generated by the function imported above from sklearn.metrics, which takes as argument the true and the predicted test labels.

The +/- in the results is obtained doubling the std\_test\_score

The function will be used to print the results for each set of parameters

```
[5]: def print results(model):
         print("Best parameters set found on train set:")
         # if best is linear there is no gamma parameter
         print(model.best_params_)
         print()
         print("Grid scores on train set:")
         means = model.cv_results_['mean_test_score']
         stds = model.cv results ['std test score']
         params = model.cv_results_['params']
         for mean, std, params_tuple in zip(means, stds, params):
             print("%0.3f (+/-%0.03f) for %r"
                   % (mean, std * 2, params_tuple))
         print()
         print("Detailed classification report for the best parameter set:")
         print("The model is trained on the full train set.")
         print("The scores are computed on the full test set.")
         print()
         y_true, y_pred = y_test, model.predict(X_test)
         print(classification_report(y_true, y_pred))
         print()
```

## 1.0.3 Loop on scores and, for each score, loop on the model labels

- iterate varying the score function
  - 1. iterate varying the classification model among Decision Tree, Naive Bayes, Linear Perceptron, Support Vector
    - activate the grid search
      - 1. the resulting model will be the best one according to the current score function
    - print the best parameter set and the results for each set of parameters using the above defined function
    - print the classification report
    - store the .best score in a dictionary for a final report
  - 2. print the final report for the current score funtion

```
[6]: results_short = {}
```

```
[7]: for score in scores:
        print('='*40)
        print("# Tuning hyper-parameters for %s" % score)
        print()
        #'%s_macro' % score ## is a string formatting expression
        # the parameter after % is substituted in the string placeholder %s
        for m in model_lbls:
            print('-'*40)
            print("Trying model {}".format(models[m]['name']))
            clf = GridSearchCV(models[m]['estimator'], models[m]['param'], cv=5,
                               scoring='%s_macro' % score,
                               iid = False,
                               return_train_score = False,
                               n_jobs = 2, # this allows using multi-cores
            clf.fit(X_train, y_train)
            print_results(clf)
            results_short[m] = clf.best_score_
        print("Summary of results for {}".format(score))
        print("Estimator")
        for m in results_short.keys():
            print("{}\t - score: {:4.2}%".format(models[m]['name'],__
     →results short[m]))
    _____
```

0.956 (+/-0.052) for  $\{'n_neighbors': 9\}$ 0.956 (+/-0.052) for  $\{'n_neighbors': 10\}$  Detailed classification report for the best parameter set:

The model is trained on the full train set.

The scores are computed on the full test set.

	precision	recall	f1-score	support
0	1.00	1.00	1.00	19
1	1.00	1.00	1.00	13
2	1.00	1.00	1.00	13
accuracy			1.00	45
macro avg	1.00	1.00	1.00	45
weighted avg	1.00	1.00	1.00	45

Estimator

K Nearest Neighbor - score: 0.96%

# Tuning hyper-parameters for recall

\_\_\_\_\_

Trying model K Nearest Neighbor
Best parameters set found on train set:

{'n\_neighbors': 8}

Grid scores on train set:

```
0.955 (+/-0.061) for {'n_neighbors': 1}
0.938 (+/-0.070) for {'n_neighbors': 2}
0.938 (+/-0.070) for {'n_neighbors': 3}
0.937 (+/-0.074) for {'n_neighbors': 4}
0.946 (+/-0.067) for {'n_neighbors': 5}
0.948 (+/-0.061) for {'n_neighbors': 6}
0.955 (+/-0.061) for {'n_neighbors': 7}
0.956 (+/-0.053) for {'n_neighbors': 8}
0.946 (+/-0.067) for {'n_neighbors': 9}
0.946 (+/-0.067) for {'n_neighbors': 10}
```

Detailed classification report for the best parameter set:

The model is trained on the full train set. The scores are computed on the full test set.

precision recall f1-score support

0	1.00	1.00	1.00	19
1	1.00	1.00	1.00	13
2	1.00	1.00	1.00	13
accuracy			1.00	45
macro avg	1.00	1.00	1.00	45
weighted avg	1.00	1.00	1.00	45

Summary of results for recall

Estimator

K Nearest Neighbor - score: 0.96%

# ml-03-04-classif-w-prepr

February 12, 2020

## 1 Preprocessing: transform categorical data

In scikit-learn the classifiers require numeric data. The library makes available a set of preprocessing fuctions which help the transformation. This exercise proposes two types of transformations:

- ullet OneHotEncoder for purely categorical columns: if the column has  ${f V}$  distinct values it is substituted by  ${f V}$  binary columns where in each row only the bit corrosponding to the original value is true
- OrdinalEncoder for ordinal columns: the original V values are mapped into the 0..V-1 range

The additional function ColumnTransformer allows to apply the different transformations to the appropriate columns with a single statement.

#### 1.0.1 To do:

- import the appropriate names
- set the random state
- import the data set with the appropriate column names
- inspect the content and the data types
- read carefully the .names file of the data set, to understand which are the ordinal and categorical data
- data cleaning
  - the ordinal transformer generates a mapping from strings to numbers according to the lexicographic sorting of the strings; in this particular case, the strings indicate numeric subranges, and ranges with one digit constitute exceptions '5-9' happens to be after '20-25'
  - it is necessary to transform '5-9' into '05-09', and the same for other similar cases
  - a way to do this is to prepare dictionaries for the translation and use the .map function
- prepare the lists of the ordinal, categorical and numeric columns
- prepare the preprocessor
- split the cleaned data into the X and y part
- fit\_transform the preprocessor and generate the transformed data set
- split the transformed data set into train and test
- use the same method used for the exercise of 19/11 to test several classifiers

```
[1]: """

http://scikit-learn.org/stable/auto_examples/model_selection/

→plot_grid_search_digits.html
```

```
Qauthor: scikit-learn.org and Claudio Sartori
11 11 11
import warnings
warnings.filterwarnings('ignore') # uncomment this line to suppress warnings
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.model selection import GridSearchCV
from sklearn.metrics import classification_report
from sklearn.metrics import confusion_matrix
from sklearn.preprocessing import OneHotEncoder, OrdinalEncoder
from sklearn.compose import ColumnTransformer
from sklearn.svm import SVC
from sklearn.linear_model import Perceptron
from sklearn.neural_network import MLPClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.naive bayes import GaussianNB
from sklearn.neighbors import KNeighborsClassifier
from sklearn.ensemble import RandomForestClassifier, AdaBoostClassifier
print( doc ) # print information included in the triple quotes at the
\rightarrow beginning
random_state = 42
```

```
http://scikit-
learn.org/stable/auto_examples/model_selection/plot_grid_search_digits.html
@author: scikit-learn.org and Claudio Sartori
```

```
[2]:
                                age menopause tumor-size inv-nodes node-caps
                                                               0-2
      no-recurrence-events
                             30-39
                                     premeno
                                                   30-34
                                                                         no
    1 no-recurrence-events
                             40-49
                                     premeno
                                                   20-24
                                                               0-2
                                                                         no
    2 no-recurrence-events
                             40-49
                                     premeno
                                                   20-24
                                                               0-2
                                                                         no
    3 no-recurrence-events
                             60-69
                                                   15-19
                                                               0-2
                                         ge40
                                                                         no
    4 no-recurrence-events
                             40-49
                                     premeno
                                                     0 - 4
                                                               0-2
                                                                         no
       deg-malig breast breast-quad irradiat
    0
                           left_low
                3
                   left
                                          no
               2 right
    1
                           right_up
                                          no
    2
                2
                           left_low
                   left
                                          no
    3
                2 right
                            left_up
                                          no
    4
                2 right
                           right_low
                                          no
    Show the types of the columns
[3]: print(df.dtypes)
    Class
                   object
                   object
    age
    menopause
                   object
    tumor-size
                   object
    inv-nodes
                   object
    node-caps
                   object
    deg-malig
                    int64
    breast
                   object
    breast-quad
                   object
    irradiat
                   object
    dtype: object
    Clean the column tumor-size
[4]: tumor_size_dict = dict(zip(list(df['tumor-size'].
     tumor_size_dict
[4]: {'30-34': '30-34',
      '20-24': '20-24',
      '15-19': '15-19',
      '0-4': '0-4',
      '25-29': '25-29',
      '50-54': '50-54',
      '10-14': '10-14',
      '40-44': '40-44',
      '35-39': '35-39',
      '5-9': '5-9',
      '45-49': '45-49'}
```

```
[5]: tumor_size_dict['0-4'] = '00-04'
      tumor_size_dict['5-9'] = '05-09'
 [6]: df['tumor-size'] = df['tumor-size'].map(tumor_size_dict)
     Clean the column inv-nodes
 [7]: | inv_nodes_dict = dict(zip(list(df['inv-nodes'].unique()),list(df['inv-nodes'].
       →unique())))
 [8]: inv_nodes_dict['0-2'] = '00-02'
      inv_nodes_dict['3-5'] = '03-05'
      inv\_nodes\_dict['6-8'] = '06-08'
      inv_nodes_dict['9-11'] = '09-11'
 [9]: df['inv-nodes'] = df['inv-nodes'].map(inv_nodes_dict)
     Inspect the data
[10]: df.head()
[10]:
                        Class
                                 age menopause tumor-size inv-nodes node-caps \
      0 no-recurrence-events 30-39
                                                     30-34
                                                               00-02
                                       premeno
                                                                            no
      1 no-recurrence-events 40-49
                                                               00-02
                                       premeno
                                                     20-24
                                                                            no
      2 no-recurrence-events 40-49
                                                     20-24
                                                               00-02
                                       premeno
                                                                            no
      3 no-recurrence-events 60-69
                                                     15-19
                                                               00-02
                                          ge40
                                                                            no
      4 no-recurrence-events 40-49
                                       premeno
                                                     00-04
                                                               00-02
                                                                            no
         deg-malig breast breast-quad irradiat
      0
                     left
                             left low
                                            no
                             right_up
      1
                 2 right
                                            no
      2
                             left_low
                 2 left
                                            no
                 2 right
      3
                             left_up
                                            no
                 2 right
                            right_low
                                            no
     Prepare the lists of numeric features, ordinal features, categorical features
[11]: categorical_features = df.dtypes.loc[df.dtypes == 'object'].index.values
      print("The non-numeric features are:")
      print(categorical_features)
     The non-numeric features are:
     ['Class' 'age' 'menopause' 'tumor-size' 'inv-nodes' 'node-caps' 'breast'
      'breast-quad' 'irradiat']
[12]: numeric_features = list(set(df.dtypes.index.values)-set(categorical_features))
      print("The numeric features are:")
      print(numeric_features)
```

```
The numeric features are:
     ['deg-malig']
[13]: ordinal_features =['age', 'tumor-size', 'inv-nodes']
      print("The ordinal features are:")
      print(ordinal_features)
     The ordinal features are:
     ['age', 'tumor-size', 'inv-nodes']
[14]: categorical_features = list(set(categorical_features) - set(ordinal_features) -
      →set(['Class']))
      print("The categorical features are:")
      print(categorical_features)
     The categorical features are:
     ['menopause', 'irradiat', 'breast', 'node-caps', 'breast-quad']
     Prepare the transformer
[15]: \# transf_dtype = np.float64
      transf_dtype = np.int32
      categorical_transformer = OneHotEncoder(handle_unknown='ignore', sparse =__
      →False, dtype = transf_dtype)
      ordinal transformer = OrdinalEncoder(dtype = transf dtype)
      preprocessor = ColumnTransformer(
          transformers = [('cat', categorical_transformer, categorical_features),
                          ('ord', ordinal transformer, ordinal features)
                          remainder = 'passthrough'
          )
     Split X and y and check the shapes
[16]: X = df.drop(['Class'], axis = 1)
      y = df['Class']
[17]: labels = y.unique()
      print("The labels are:")
      print(labels)
     The labels are:
     ['no-recurrence-events' 'recurrence-events']
[18]: X.shape
[18]: (286, 9)
```

Fit the preprocessor with X and check the parameters printing the .named\_transformers\_ attribute

[19]: preprocessor.fit(X)

```
[19]: ColumnTransformer(n_jobs=None, remainder='passthrough', sparse_threshold=0.3,
                        transformer_weights=None,
                        transformers=[('cat',
                                        OneHotEncoder(categorical_features=None,
                                                       categories=None, drop=None,
                                                       dtype=<class 'numpy.int32'>,
                                                       handle unknown='ignore',
                                                       n values=None, sparse=False),
                                        ['menopause', 'irradiat', 'breast',
                                          'node-caps', 'breast-quad']),
                                       ('ord',
                                        OrdinalEncoder(categories='auto',
                                                        dtype=<class 'numpy.int32'>),
                                        ['age', 'tumor-size', 'inv-nodes'])],
                        verbose=False)
[20]: print(preprocessor.named_transformers_)
     {'cat': OneHotEncoder(categorical_features=None, categories=None, drop=None,
                    dtype=<class 'numpy.int32'>, handle unknown='ignore',
                    n_values=None, sparse=False), 'ord':
     OrdinalEncoder(categories='auto', dtype=<class 'numpy.int32'>), 'remainder':
      'passthrough'}
     Fit-transform X and store the result in X p, check the shape
[21]: X_p = preprocessor.fit_transform(X)
[22]: X_p.shape
[22]: (286, 20)
     For ease of inspection transform X_p into a data frame df_p and inspect it
[23]: df_p = pd.DataFrame(X_p)
[24]: df p.describe()
[24]:
                                              2
                                                           3
                     0
                                  1
                                                                                    5
             286.000000
                         286.000000
                                      286.000000
                                                  286.000000
                                                               286.000000
                                                                           286.000000
      count
               0.451049
                            0.024476
                                        0.524476
                                                     0.762238
                                                                 0.237762
                                                                              0.531469
      mean
      std
               0.498470
                            0.154791
                                        0.500276
                                                     0.426459
                                                                 0.426459
                                                                              0.499883
               0.000000
                            0.000000
                                        0.000000
                                                     0.000000
                                                                 0.000000
                                                                              0.00000
      min
      25%
               0.000000
                            0.000000
                                        0.000000
                                                     1.000000
                                                                 0.000000
                                                                              0.00000
```

	50%	/.		0	000	000		0	იიი	000		1 0	0000	0	1 (	0000	0	0 0	0000	00	1 0	00000	)
	ວວ, 75%					000				000			0000			0000			00000			00000	
	max					000				000			0000			0000			0000			00000	
•	maz			٠.	000	,000		٠.	000	000		1.0	0000	O	1.0	,0000	O	1.0	,0000	, ,	1.0	00000	•
						6				7			8			9			1	.0		11	. \
	cou	ınt	2	86.	000	000	2	86.	000	000	2	86.0	0000	0 2	286.0	0000	0 2	286.0	00000	00 2	286.0	00000	)
1	mea	an		0.	468	531		0.	027	972		0.7	7622	4	0.1	9580	4	0.0	0349	7	0.0	73427	•
:	sto	i		0.	499	883		0.	165	182		0.4	1750	4	0.3	9751	4	0.0	5913	31	0.2	61293	}
1	mir	ı		0.	000	000		0.	000	000		0.0	0000	0	0.0	0000	0	0.0	0000	0	0.0	00000	)
:	25%	<b>/</b>		0.	000	000		0.	000	000		1.0	0000	0	0.0	0000	0	0.0	0000	0	0.0	00000	)
į	50%	<b>/</b>		0.	000	000		0.	000	000		1.0	0000	0	0.0	0000	0	0.0	0000	0	0.0	00000	)
	75%	<b>/</b>		1.	000	000		0.	000	000		1.0	0000	0	0.0	0000	0	0.0	0000	0	0.0	00000	)
	max			1.	000	000		1.	000	000		1.0	0000	0	1.0	0000	0	1.0	0000	0	1.0	00000	)
						12				13			1	4		1	5		1	.6		17	. \
	cou	ınt	2	86.	000	000	2	86.	000	000	2	86.0	0000	0 2	286.0	0000	0 2	286.0	0000	00 2	286.0	00000	)
1	mea	an		0.	384	615		0.	339	161		0.0	8391	6	0.1	1538	5	2.6	6433	86	4.8	81119	)
	sto	i		0.	487	357		0.	474	254		0.2	7774	8	0.3	2004	6	1.0	1181	.8	2.1	05930	)
1	mir	ı		0.	000	000		0.	000	000		0.0	0000	0	0.0	0000	0	0.0	0000	0	0.0	00000	)
:	25%	<b>/</b>		0.	000	000		0.	000	000		0.0	0000	0	0.0	0000	0	2.0	0000	0	4.0	00000	)
į	50%	<b>/</b>		0.	000	000		0.	000	000		0.0	0000	0	0.0	0000	0	3.0	0000	0	5.0	00000	)
	75%	<b>/</b>		1.	000	000		1.	000	000		0.0	0000	0	0.0	0000	0	3.0	0000	0	6.0	00000	)
1	max	ζ		1.	000	000		1.	000	000		1.0	0000	0	1.0	0000	0	5.0	0000	0	10.0	00000	)
						18				19													
	cou	ınt	2	86.	000	000	2	86.	000	000													
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:	sto	i		1.	110	417		0.	738	217													
1	mir	ı		0.	000	000		1.	000	000													
:	25%	<b>/</b>		0.	000	000		2.	000	000													
	50%	<b>/</b>		0.	000	000		2.	000	000													
•	75%	<b>/</b>		1.	000	000		3.	000	000													
]	max	ζ		6.	000	000		3.	000	000													
	df_	_p.	hea	.d()																			
:		0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19		
(	0	0	0	1	1	0	1		0	1	0	0	0	1	0	0	0	1	6	0	3		
	1	0	0	1			0	1			0	0	0	0	0	0	1	2	4	0	2		

The columns in the transformed dataset are generated according to the order you see printing the preprocessor after fitting, therefore the last four columns correspond to 'age', 'tumor-size', 'inv-nodes', 'deg-malig'.

[25]:

[25]:

0 0 1 0 1

In order to inspect if the translation and check if the mapping is as expected, compare the sorted

values of df['tumor-size'] and df\_p[17], e.g. comparing the index sequences

The number of index discordances between 'tumor-size' and '17' is 0  $\frac{1}{2}$  Train/test split

```
[27]: X_train, X_test, y_train, y_test = train_test_split(X_p,y, random_state = □ → random_state)
```

Classification and test

```
[28]: model_lbls = [
                   'dt'.
                   'nb',
                   'lp',
                    'svc',
                    'knn',
                   'rfc'.
                   'ada',
      # Set the parameters by cross-validation
      tuned_param_dt = [{'max_depth': list(range(1,20))}]
      tuned param nb = [\{'var smoothing': [10**i for i in range(1,-11, -1)]\}]
      tuned_param_lp = [{'early_stopping': [True]}]
      tuned_param_svc = [{'kernel': ['rbf'],
                           'gamma': [1e-3, 1e-4],
                             'C': [1, 10, 100, 1000],
      #
                           'C': [10**i for i in range(0,4)],
                          {'kernel': ['linear'],
                          'C': [10**i for i in range(0,4)],
                          },
      tuned_param_knn =[{'n_neighbors': list(range(1,11)),
                          'metric': ['euclidean', 'manhattan', 'chebyshev']}
      tuned_param_rfc = [{'max_depth': list(range(1,11))}]
      tuned_param_ada = [{'learning_rate': [1., 0.1, 0.01, 0.001, 0.0001]}]
      models = {
          'dt': {'name': 'Decision Tree
```

```
'estimator': DecisionTreeClassifier(),
           'param': tuned_param_dt,
          },
    'nb': {'name': 'Gaussian Naive Bayes',
           'estimator': GaussianNB(),
           'param': tuned_param_nb
    'lp': {'name': 'Linear Perceptron',
           'estimator': Perceptron(),
           'param': tuned_param_lp,
          },
    'svc':{'name': 'Support Vector
           'estimator': SVC(),
           'param': tuned_param_svc
          },
    'knn':{'name': 'K Nearest Neighbor ',
           'estimator': KNeighborsClassifier(),
           'param': tuned_param_knn
          },
    'rfc':{'name': 'Random Forest
           'estimator': RandomForestClassifier(),
           'param': tuned_param_rfc
          },
    'ada':{'name': 'Adaboost
           'estimator': AdaBoostClassifier(),
           'param': tuned param ada
          },
}
scores = [
     'precision_macro',
    'recall_macro',
#
    'accuracy',
#
     'f1_macro'
]
```

```
[29]: # def plot_confusion_matrix(cm):
           print(cm)
      #
           fig = plt.figure(figsize=(10,10))
      #
           ax = fiq.add\_subplot(111)
            cax = ax.matshow(cm)
      #
            plt.title('Confusion matrix of the classifier')
      #
      #
           fig.colorbar(cax)
      #
           ax.set_xticklabels([''] + labels)
      #
           ax.set_yticklabels([''] + labels)
      #
            plt.xlabel('Predicted')
            plt.ylabel('True')
```

```
plt.show()
def print_results(model):
    print("Best parameters set found on train set:")
    print()
    # if best is linear there is no gamma parameter
    print(model.best_params_)
    print()
    print("Grid scores on train set:")
    means = model.cv_results_['mean_test_score']
    stds = model.cv_results_['std_test_score']
    params = model.cv_results_['params']
    for mean, std, params_tuple in zip(means, stds, params):
        print("%0.3f (+/-%0.03f) for %r"
              % (mean, std * 2, params_tuple))
    print()
    print("Detailed classification report for the best parameter set:")
    print()
    print("The model is trained on the full train set.")
    print("The scores are computed on the full test set.")
    print()
    y_true, y_pred = y_test, model.predict(X_test)
    print(classification_report(y_true, y_pred))
    cm = confusion_matrix(y_true,y_pred, labels = labels)
   print(cm)
     plot_confusion_matrix(cm)
    print()
```

```
clf.fit(X_train, y_train)
        print_results(clf)
        results_short[m] = clf.best_score_
    print("Summary of results for {}".format(score))
    print("Estimator")
    for m in results_short.keys():
        print("{}\t - score: {:4.2}%".format(models[m]['name'],_
 →results_short[m]))
# Tuning hyper-parameters for recall_macro
Trying model Decision Tree
Best parameters set found on train set:
{'max_depth': 14}
Grid scores on train set:
0.567 (+/-0.086) for {'max_depth': 1}
0.610 (+/-0.115) for {'max_depth': 2}
0.583 (+/-0.127) for {\max_depth': 3}
0.551 (+/-0.082) for {'max_depth': 4}
0.574 (+/-0.148) for {\max_{depth': 5}}
0.574 (+/-0.138) for {'max_depth': 6}
0.597 (+/-0.148) for {\max_{depth'}: 7}
0.591 (+/-0.226) for {'max_depth': 8}
0.567 (+/-0.223) for {'max_depth': 9}
0.576 \ (+/-0.285) \ for \ {'max_depth': 10}
0.577 (+/-0.168) for {'max_depth': 11}
0.552 (+/-0.166) for {'max_depth': 12}
0.564 (+/-0.163) for {'max_depth': 13}
0.620 (+/-0.187) for {'max_depth': 14}
0.565 (+/-0.142) for {'max_depth': 15}
0.573 (+/-0.089) for {'max_depth': 16}
0.608 (+/-0.121) for {'max_depth': 17}
0.571 (+/-0.154) for {'max_depth': 18}
0.576 (+/-0.177) for {'max_depth': 19}
Detailed classification report for the best parameter set:
The model is trained on the full train set.
The scores are computed on the full test set.
                      precision
                                 recall f1-score
                                                      support
```

no-recurrence-events	0.72	0.84	0.77	49
recurrence-events	0.47	0.30	0.37	23
accuracy			0.67	72
macro avg	0.59	0.57	0.57	72
weighted avg	0.64	0.67	0.64	72

[[41 8] [16 7]]

-----

Trying model Gaussian Naive Bayes
Best parameters set found on train set:

{'var\_smoothing': 0.01}

Grid scores on train set:

```
0.500 (+/-0.000) for {'var_smoothing': 10}
0.506 (+/-0.049) for {'var_smoothing': 1}
0.593 (+/-0.115) for {'var_smoothing': 0.1}
0.629 (+/-0.134) for {'var_smoothing': 0.01}
0.627 (+/-0.125) for {'var_smoothing': 0.001}
0.624 (+/-0.121) for {'var_smoothing': 0.0001}
0.611 (+/-0.076) for {'var_smoothing': 1e-05}
0.601 (+/-0.092) for {'var_smoothing': 1e-06}
0.591 (+/-0.094) for {'var_smoothing': 1e-07}
0.577 (+/-0.124) for {'var_smoothing': 1e-08}
0.556 (+/-0.142) for {'var_smoothing': 1e-09}
0.551 (+/-0.135) for {'var_smoothing': 1e-10}
```

Detailed classification report for the best parameter set:

The model is trained on the full train set. The scores are computed on the full test set.

	precision	recall	f1-score	support
no-recurrence-events	0.73	0.88	0.80	49
recurrence-events	0.54	0.30	0.39	23
accuracy			0.69	72
macro avg	0.63	0.59	0.59	72
weighted avg	0.67	0.69	0.67	72

[[43 6] [16 7]] -----

Trying model Linear Perceptron
Best parameters set found on train set:

{'early\_stopping': True}

Grid scores on train set:

0.564 (+/-0.111) for {'early\_stopping': True}

Detailed classification report for the best parameter set:

The model is trained on the full train set. The scores are computed on the full test set.

	precision	recall	f1-score	support
no-recurrence-events	1.00	0.14	0.25	49
recurrence-events	0.35	1.00	0.52	23
accuracy			0.42	72
macro avg	0.68	0.57	0.39	72
weighted avg	0.79	0.42	0.34	72

[[ 7 42] [ 0 23]]

-----

Trying model Support Vector
Best parameters set found on train set:

{'C': 10, 'kernel': 'linear'}

Grid scores on train set:

```
0.500 (+/-0.000) for {'C': 1, 'gamma': 0.001, 'kernel': 'rbf'}
0.500 (+/-0.000) for {'C': 1, 'gamma': 0.0001, 'kernel': 'rbf'}
0.495 (+/-0.048) for {'C': 10, 'gamma': 0.001, 'kernel': 'rbf'}
0.500 (+/-0.000) for {'C': 10, 'gamma': 0.0001, 'kernel': 'rbf'}
0.549 (+/-0.064) for {'C': 100, 'gamma': 0.001, 'kernel': 'rbf'}
0.495 (+/-0.048) for {'C': 100, 'gamma': 0.001, 'kernel': 'rbf'}
0.574 (+/-0.122) for {'C': 1000, 'gamma': 0.001, 'kernel': 'rbf'}
0.574 (+/-0.074) for {'C': 1000, 'gamma': 0.0001, 'kernel': 'rbf'}
0.582 (+/-0.091) for {'C': 1, 'kernel': 'linear'}
0.599 (+/-0.159) for {'C': 10, 'kernel': 'linear'}
0.599 (+/-0.159) for {'C': 100, 'kernel': 'linear'}
0.599 (+/-0.159) for {'C': 100, 'kernel': 'linear'}
```

Detailed classification report for the best parameter set:

The model is trained on the full train set. The scores are computed on the full test set.

	precision	recall	f1-score	support
no-recurrence-events	0.73	0.92	0.81	49
recurrence-events	0.60	0.26	0.36	23
accuracy			0.71	72
macro avg	0.66	0.59	0.59	72
weighted avg	0.69	0.71	0.67	72

[[45 4] [17 6]]

-----

Trying model K Nearest Neighbor
Best parameters set found on train set:

{'metric': 'manhattan', 'n\_neighbors': 7}

## Grid scores on train set:

```
0.567 (+/-0.088) for {'metric': 'euclidean', 'n_neighbors': 1}
0.524 (+/-0.037) for {'metric': 'euclidean', 'n_neighbors': 2}
0.554 (+/-0.190) for {'metric': 'euclidean', 'n_neighbors': 3}
0.542 (+/-0.104) for {'metric': 'euclidean', 'n_neighbors': 4}
0.548 (+/-0.115) for {'metric': 'euclidean', 'n_neighbors': 5}
0.502 (+/-0.075) for {'metric': 'euclidean', 'n_neighbors': 6}
0.555 (+/-0.096) for {'metric': 'euclidean', 'n_neighbors': 7}
0.523 (+/-0.080) for {'metric': 'euclidean', 'n_neighbors': 8}
0.521 (+/-0.091) for {'metric': 'euclidean', 'n_neighbors': 9}
0.524 (+/-0.079) for {'metric': 'euclidean', 'n neighbors': 10}
0.578 (+/-0.077) for {'metric': 'manhattan', 'n_neighbors': 1}
0.554 (+/-0.063) for {'metric': 'manhattan', 'n neighbors': 2}
0.554 (+/-0.170) for {'metric': 'manhattan', 'n_neighbors': 3}
0.570 (+/-0.086) for {'metric': 'manhattan', 'n_neighbors': 4}
0.562 (+/-0.052) for {'metric': 'manhattan', 'n_neighbors': 5}
0.553 (+/-0.097) for {'metric': 'manhattan', 'n_neighbors': 6}
0.584 (+/-0.124) for {'metric': 'manhattan', 'n_neighbors': 7}
0.566 (+/-0.158) for {'metric': 'manhattan', 'n_neighbors': 8}
0.560 (+/-0.161) for {'metric': 'manhattan', 'n_neighbors': 9}
0.561 (+/-0.095) for {'metric': 'manhattan', 'n_neighbors': 10}
0.490 (+/-0.152) for {'metric': 'chebyshev', 'n_neighbors': 1}
0.521 (+/-0.128) for {'metric': 'chebyshev', 'n_neighbors': 2}
0.575 (+/-0.146) for {'metric': 'chebyshev', 'n_neighbors': 3}
```

```
0.539 (+/-0.090) for {'metric': 'chebyshev', 'n_neighbors': 4} 0.576 (+/-0.095) for {'metric': 'chebyshev', 'n_neighbors': 5} 0.518 (+/-0.087) for {'metric': 'chebyshev', 'n_neighbors': 6} 0.531 (+/-0.100) for {'metric': 'chebyshev', 'n_neighbors': 7} 0.518 (+/-0.068) for {'metric': 'chebyshev', 'n_neighbors': 8} 0.520 (+/-0.086) for {'metric': 'chebyshev', 'n_neighbors': 9} 0.539 (+/-0.070) for {'metric': 'chebyshev', 'n_neighbors': 10}
```

Detailed classification report for the best parameter set:

The model is trained on the full train set. The scores are computed on the full test set.

	precision	recall	f1-score	support
	_			
no-recurrence-events	0.69	0.92	0.79	49
recurrence-events	0.43	0.13	0.20	23
accuracy			0.67	72
macro avg	0.56	0.52	0.49	72
weighted avg	0.61	0.67	0.60	72

[[45 4] [20 3]]

-----

Trying model Random Forest
Best parameters set found on train set:

{'max\_depth': 8}

Grid scores on train set:

```
0.533 (+/-0.082) for {'max_depth': 1}

0.604 (+/-0.076) for {'max_depth': 2}

0.587 (+/-0.130) for {'max_depth': 3}

0.595 (+/-0.111) for {'max_depth': 4}

0.599 (+/-0.194) for {'max_depth': 5}

0.590 (+/-0.115) for {'max_depth': 6}

0.580 (+/-0.117) for {'max_depth': 7}

0.614 (+/-0.110) for {'max_depth': 8}

0.560 (+/-0.087) for {'max_depth': 9}

0.600 (+/-0.112) for {'max_depth': 10}
```

Detailed classification report for the best parameter set:

The model is trained on the full train set.

The scores are computed on the full test set.

	precision	recall	f1-score	support
	•			••
no-recurrence-events	0.73	0.96	0.83	49
recurrence-events	0.75	0.26	0.39	23
accuracy			0.74	72
macro avg	0.74	0.61	0.61	72
weighted avg	0.74	0.74	0.69	72

[[47 2] [17 6]]

-----

Trying model Adaboost

Best parameters set found on train set:

{'learning\_rate': 0.01}

Grid scores on train set:

0.586 (+/-0.146) for {'learning\_rate': 1.0} 0.620 (+/-0.102) for {'learning\_rate': 0.1} 0.643 (+/-0.161) for {'learning\_rate': 0.01} 0.567 (+/-0.086) for {'learning\_rate': 0.001} 0.567 (+/-0.086) for {'learning\_rate': 0.0001}

Detailed classification report for the best parameter set:

The model is trained on the full train set. The scores are computed on the full test set.

	precision	recall	f1-score	support
no-recurrence-events	0.72	0.98	0.83	49
recurrence-events	0.80	0.17	0.29	23
accuracy			0.72	72
macro avg	0.76	0.58	0.56	72
weighted avg	0.74	0.72	0.65	72

[[48 1] [19 4]]

Summary of results for recall\_macro

Estimator

Decision Tree - score: 0.62% Gaussian Naive Bayes - score: 0.63% Linear Perceptron - score: 0.56%
Support Vector - score: 0.6%
K Nearest Neighbor - score: 0.58%
Random Forest - score: 0.61%
Adaboost - score: 0.64%

## ml-04-ex1-KMeans-elbow

February 12, 2020

Claudio Sartori

Elaboration from the example given in Sebastian Raschka, 2015 https://github.com/rasbt/python-machine-learning-book

## 1 Machine Learning - Lab

- 1.1 Working with Unlabeled Data Clustering Analysis
- 1.1.1 Find the best number of clusters with k\_means
- 1.1.2 Overview
  - Section 2
  - Section 2.1
  - Section 2.2

```
[1]: from IPython.display import Image
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score, silhouette_samples

%matplotlib inline

rnd_state = 42 # This variable will be used in all the procedure calls allowing
→ a random_state parameter

# in this way the running can be perfectly reproduced
# just change this value for a different experiment
```

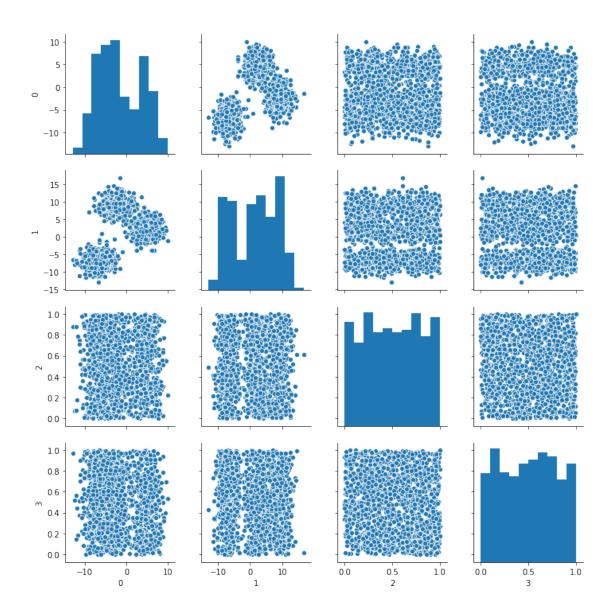
# 2 Grouping objects by similarity using k-means

In this example we will use an artificial data set

- 1. load the data file from 'ex1\_4dim\_data.csv'
- 2. check the shape and plot the content
- 3. observe the plot and decide which are the most interesting columns, to use in the plots of the clusters
- make a 2d plot of the two most promising columns
- 4. Use the elbow method to find the optimal number of clusters: test KMeans with varying number of clusters, from 2 to 10, fitting the data and computing the inertia and the silhouette score
- 5. Choose the optimal number of clusters looking at the plots, then cluster the data, plot the clusters and plot the scores of the individual samples
- 6. For comparison, repeat 5 with two clusters

```
[2]: data_file = 'ex1_4dim_data.csv'
delimiter = ','
X = np.loadtxt(data_file, delimiter = delimiter)
```

- [3]: X.shape
- [3]: (1500, 4)
- [4]: sns.pairplot(pd.DataFrame(X))
- [4]: <seaborn.axisgrid.PairGrid at 0x1a242bbfd0>



### 2.0.1 3. Observe the pairplots

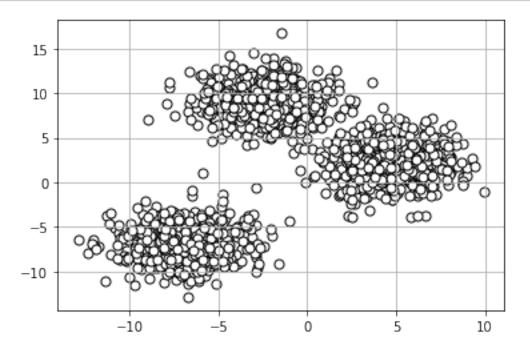
In this simple example you can easily see that the two most interesting columns are 0 and 1.

```
[5]: focus = [0,1]
plt.scatter(X[:,focus[0]], X[:,focus[1]]

, c='white'  # color filling the data markers
, edgecolors='black' # edge color for data markers
, marker='o'  # data marker shape, e.g. triangles (v<>^),⊔

→square (s), star (*), ...
, s=50)  # data marker size
plt.grid() # plots a grid on the data
```

### plt.show()



# [6]: from plot\_clusters import plot\_clusters

## [7]: help(plot\_clusters)

Help on function plot\_clusters in module plot\_clusters:

plot\_clusters(X, y, dim, points, labels\_prefix='cluster',
points\_name='centroids', colors=<matplotlib.colors.ListedColormap object at
0x11b0e5b50>, points\_color=(0.09019607843137255, 0.7450980392156863,
0.8117647058823529, 1.0))

Plot a two dimensional projection of an array of labelled points

X: array with at least two columns

y: vector of labels, length as number of rows in X

dim: the two columns to project, inside range of X columns, e.g. (0,1)

points: additional points to plot as 'stars'

labels\_prefix: prefix to the labels for the legend ['cluster']

points name: legend name for the additional points ['centroids']

colors: a color map

points\_color: the color for the points

### 2.1 Using the elbow method to find the optimal number of clusters

We will try **k\_means** with a number of clusters varying from 2 to 10

- prepare two emptys lists for inertia and silhouette scores
- For each value of the number of clusters:
- initialize an estimator for KMeans and fit\_predict
- we will store the distortion (from the fitted model) in the variable distortions
- using the function silhouette\_score from sklearn.metrics with arguments the data and the fitted labels, we will fill the variable silhouette\_scores

Then we will plot the two lists in the y axis, with the range of k in the x axis. The plot with two different scales in the y axis can be done according to the example shown in the notebook two\_scales.ipynb.

```
[8]: k_range = range(2,11)
```

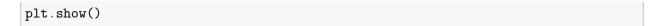
```
[10]: fig, ax1 = plt.subplots()

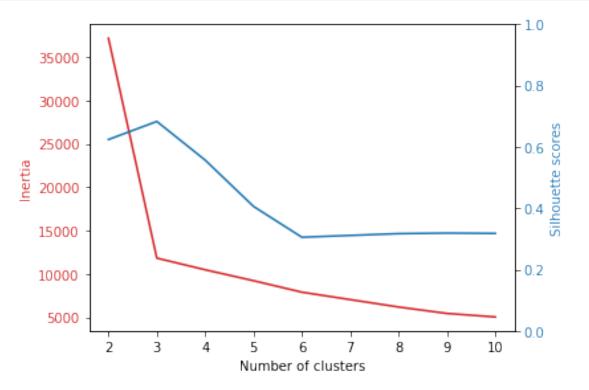
color = 'tab:red'
ax1.set_xlabel('Number of clusters')
ax1.set_ylabel('Inertia', color=color)
ax1.plot(k_range, distortions, color=color)
ax1.tick_params(axis='y', labelcolor=color)

ax2 = ax1.twinx()  # instantiate a second axes that shares the same x-axis

color = 'tab:blue'
ax2.set_ylabel('Silhouette scores', color=color)  # we already handled the_u
-x-label with ax1
ax2.plot(k_range, silhouette_scores, color=color)
ax2.tick_params(axis='y', labelcolor=color)
ax2.set_ylim(0,1)  # the axis for silhouette is [0,1]

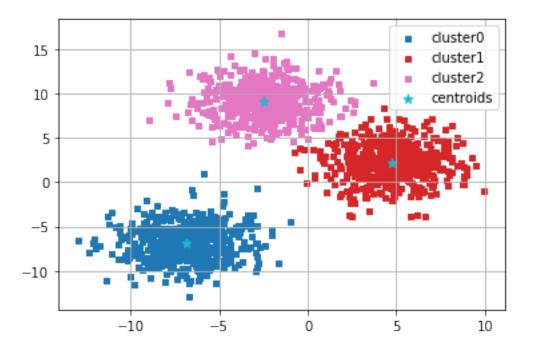
fig.tight_layout()  # otherwise the right y-label is slightly clipped
```





### 2.1.1 5. Cluster with the optimal number

```
[11]: good_k = 3
[12]: km = KMeans(n_clusters=good_k,
                  init='k-means++',
                  n_init=10,
                 max_iter=300,
                  tol=1e-04,
                  random_state=rnd_state)
      y_km = km.fit_predict(X)
[13]: km.cluster_centers_
[13]: array([[-6.89370123, -6.83658926, 0.52620605,
                                                      0.52371904],
             [ 4.75108211, 2.11850327,
                                        0.4917521 ,
                                                      0.49502881],
             [-2.50474216, 9.09132188,
                                         0.49394552,
                                                      0.48136246]])
[14]: plot_clusters(X,y_km,dim=(focus[0],focus[1]), points = km.cluster_centers_)
```



[15]: print('Distortion: %.2f' % km.inertia\_)

Distortion: 11831.85

### 2.2 Quantifying the quality of clustering via silhouette plots

The silhouette scores for the individual samples are computed with the function silhouette samples

The function plot\_silhouette produces a 'horizontal bar-plot', with one bar for each sample, where the length of the bar is proportional to the silhouette score of the sample. The bars are grouped for cluster and sorted for decreasing length.

A vertical line represents the silhouette score, i.e. the average on all the samples,

[16]: # from plot\_silhouette import plot\_silhouette
from plot\_silhouette2 import plot\_silhouette

[17]: help(plot\_silhouette)

Help on function plot\_silhouette in module plot\_silhouette2:

plot\_silhouette(silhouette\_vals, y, colors=<matplotlib.colors.ListedColormap
object at 0x11b0e5b50>, plot\_noise=False)

Plotting silhouette scores for the individual samples of a labelled data set.

The scores will be grouped according to labels and sorted in descending

order.

The bars are proportional to the score and the color is determined by the label.

silhouette\_vals: the silhouette values of the samples

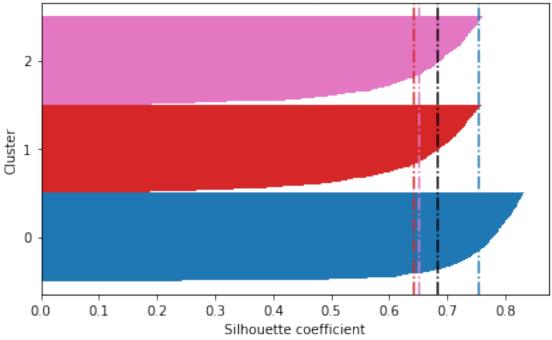
y: the labels of the samples

plot\_noise: boolean, assumes the noise to be labeled with a negative

integer

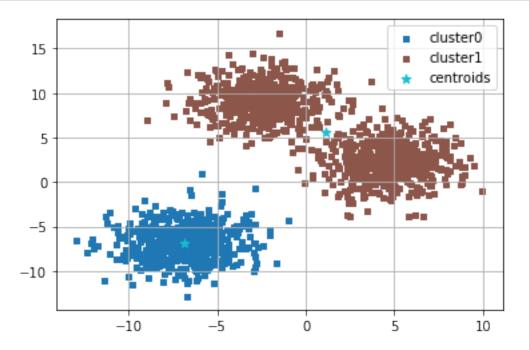
```
[18]: cluster_labels = np.unique(y_km)
    n_clusters = cluster_labels.shape[0] # it is the number of rows
# Compute the Silhouette Coefficient for each sample, with the euclidean metric
silhouette_score_samples = silhouette_samples(X, y_km, metric='euclidean')
plt.title('Silhouette score for samples with {} clusters'.format(good_k))
plot_silhouette(silhouette_score_samples, y_km)
```



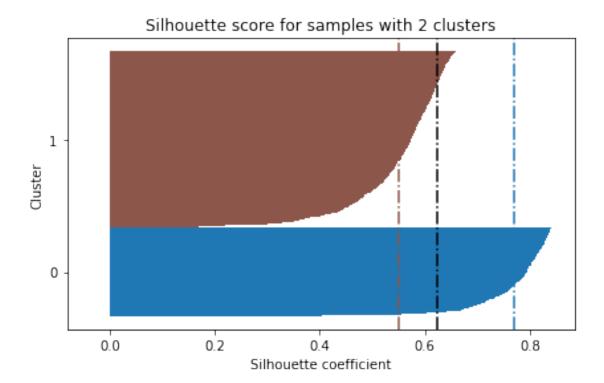


### 2.2.1 6. Comparison to "bad" clustering:

[19]: bad\_k = 2



```
[21]: cluster_labels = np.unique(y_km)
    n_clusters = cluster_labels.shape[0]
    silhouette_score_samples = silhouette_samples(X, y_km, metric='euclidean')
    plt.title('Silhouette score for samples with {} clusters'.format(bad_k))
    plot_silhouette(silhouette_score_samples, y_km)
```



[]:

### ml-04-ex2-dbscan

February 12, 2020

#### Claudio Sartori

Elaboration from the example given in Sebastian Raschka, 2015

https://github.com/rasbt/python-machine-learning-book

## 1 Machine Learning - Lab

## 1.1 Working with Unlabeled Data – Clustering Analysis

#### 1.1.1 Use DBSCAN

#### 1.1.2 Overview

In this example we will use an artificial data set

- 1. load the data
- 2. check the shape and plot the content
- 3. observe the plot and decide which are the most interesting columns, to use in the plots of the clusters
- make a 2d plot of the two most promising columns
- use the 2d projection only for plotting, not for the other computations 4. initialize and fit\_predict an estimator for DBSCAN, using the default parameters, then print the results print the estimator to check the parameter values
- the labels are the unique values of the predicted values
- print if there is noise
- if there is noise the first cluster label will be -1
- print the number of clusters (noise excluded)
- the other clusters are labeled starting from 0
- for each cluster (noise excluded) compute the centroid
- plot the data with the centroids and the colors representing clusters
- use the plot\_clusters function provided
- 5. find the best parameters using ParameterGrid prepare a dictionary with the parameters lists
- generate the list of the parameter combinations with  ${\tt ParameterGrid}$  for each combination of parameters
- initialize the DBSCAN estimator
- fit\_predict
- extract the labels and the number of clusters excluding the *noise*
- compute the silhouette score and the number of unclustered objects (noise)

- filter and print the parameters and the results
- print if the silhouette score is above a threshold and the percentage of unclustered is below a threshold
- 6. observe visually the most promising combination of parameters
- fit and predict the estimator
- plot the clusters
- compute the silouette scores for the individual samples using the function silhouette\_samples
- plot the silhouette scores for each sample using the function plot\_silhouette

```
[1]: from IPython.display import Image
     import numpy as np
     import matplotlib.pyplot as plt
     import seaborn as sns
     import pandas as pd
     from sklearn.cluster import DBSCAN
     from sklearn.metrics import silhouette_score, silhouette_samples
     from sklearn.preprocessing import MinMaxScaler
     from sklearn.model_selection import ParameterGrid
     from sklearn.preprocessing import MinMaxScaler
     %matplotlib inline
     rnd_state = 42 # This variable will be used in all the procedure calls allowing_
     \rightarrowa random state parameter
                    # in this way the running can be perfectly reproduced
                    # just change this value for a different experiment
     # the .py files with the functions provided must be in the same directory of \Box
     \hookrightarrow the .ipynb file
     from plot clusters import plot clusters # python script provided separately
     from plot_silhouette import plot_silhouette # python script provided separately
```

#### [2]: help(plot\_clusters)

Help on function plot\_clusters in module plot\_clusters:

points\_color: the color for the points

### [3]: help(plot\_silhouette)

Help on function plot\_silhouette in module plot\_silhouette:

plot\_silhouette(silhouette\_vals, y, colors=<matplotlib.colors.ListedColormap
object at 0x11ebcb210>, plot\_noise=False)

Plotting silhouette scores for the individual samples of a labelled data set.

The scores will be grouped according to labels and sorted in descending order.

The bars are proportional to the score and the color is determined by the label.

```
silhouette_vals: the silhouette values of the samples
y: the labels of the samples
plot_noise: boolean, assumes the noise to be labeled with a negative
integer
```

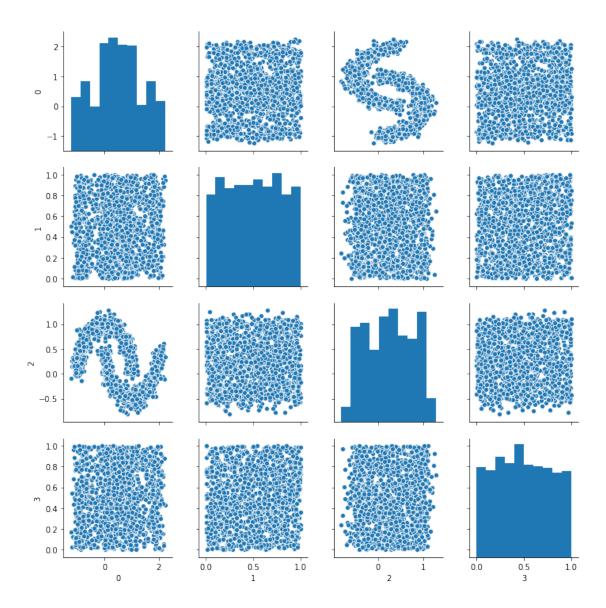
#### 1.1.3 1. Load the data

```
[4]: # data_file = 'ex1_4dim_data.csv'
# data_file = 'ex1_4dim_mod_data.csv'
# data_file = 'ex1_data.csv'
data_file = 'ex1_4d_moon.csv'
delimiter = ','
X = np.loadtxt(data_file, delimiter = delimiter)
# scaler = MinMaxScaler()
# X = scaler.fit_transform(X)
```

### 1.1.4 2. Inspect

```
[5]: X.shape
[5]: (1500, 4)
[6]: sns.pairplot(pd.DataFrame(X))
```

[6]: <seaborn.axisgrid.PairGrid at 0x1a2414bb90>



### 1.1.5 3. Observing the pairplots

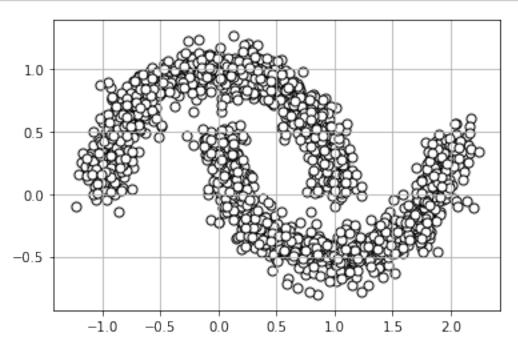
In this simple example you can easily see which are the two most interesting columns.

All the plots will focus on those columns

```
[7]: # focus = [0,1]
focus = [0,2]
plt.scatter(X[:,focus[0]], X[:,focus[1]]
, c='white' # color filling the data markers
, edgecolors='black' # edge color for data markers
, marker='o' # data marker shape, e.g. triangles (v<>^), u

square (s), star (*), ...
```

```
, s=50) # data marker size
plt.grid() # plots a grid on the data
plt.show()
```



### 1.1.6 4. Initialize, fit\_predict and plot the clusters

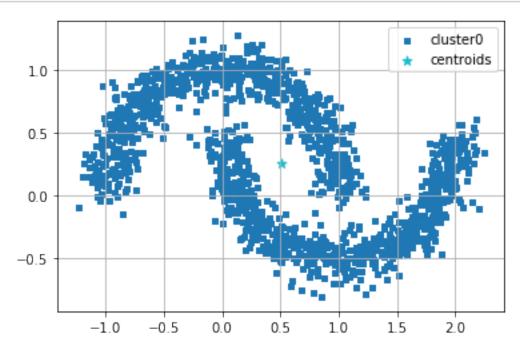
```
[8]: db = DBSCAN()
y_db = db.fit_predict(X)
```

[9]: print(db)

```
[10]: cluster_labels_all = np.unique(y_db)
    cluster_labels = cluster_labels_all[cluster_labels_all != -1]
    n_clusters = len(cluster_labels)
    if cluster_labels_all[0] == -1:
        noise = True
        print("There is noise")
    else:
        noise = False
    print("There is/are {} cluster(s)".format(n_clusters-noise))
```

There is/are 1 cluster(s)

```
[11]: cluster_centers = np.empty((n_clusters, X.shape[1]))
    for i in cluster_labels:
        cluster_centers[i,:] = np.mean(X[y_db==i,:], axis = 0)
    plot_clusters(X,y_db,dim=(focus[0],focus[1]), points = cluster_centers)
```



#### 1.1.7 5. Find the best parameters using ParameterGrid

eps	$min_samples$	n_clusters	silhouette	unclust%
0.05	1	1490	0.01	0.00%
0.10	1	1297	0.09	0.00%
0.15	1	698	0.07	0.00%
0.15	2	253	0.25	29.67%
0.25	2	2	0.14	1.27%
0.25	7	2	0.28	3.27%
0.25	8	2	0.28	5.80%
0.25	9	2	0.29	8.47%

#### 1.1.8 6. Observe

- Observe visually the most promising combination of parameters.
- Plot the clusters with the centers
- Plot the silhouette indexs for all the clustered samples

```
[14]: # db = DBSCAN(eps=0.9, min_samples=4)
db = DBSCAN(eps=0.25, min_samples=9)
y_db = db.fit_predict(X)
cluster_labels_all = np.unique(y_db)
cluster_labels = cluster_labels_all[cluster_labels_all != -1]
n_clusters = len(cluster_labels)
```

```
[15]: cluster_centers = np.empty((n_clusters,X.shape[1]))
for i in cluster_labels:
    cluster_centers[i,:] = np.mean(X[y_db==i,:], axis = 0)
```

```
[16]: print("There are {} clusters".format(n_clusters))
```

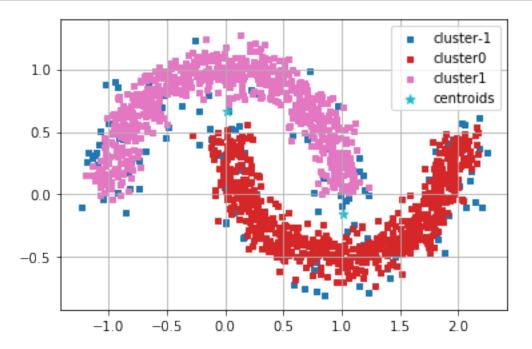
There are 2 clusters

```
[17]: print("The cluster labels are {}".format(cluster_labels))
```

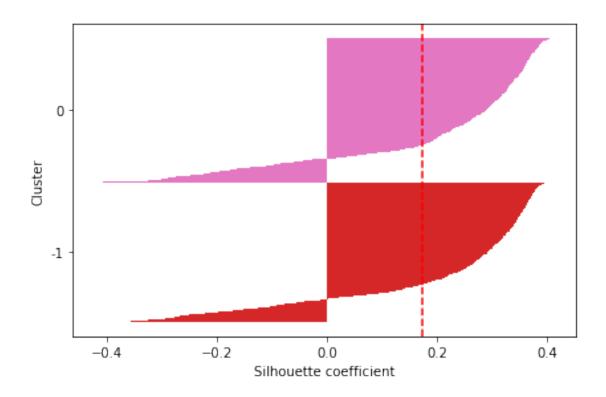
The cluster labels are [0 1]

```
[18]: cluster_centers
```

```
[19]: plot_clusters(X,y_db,dim=(focus[0],focus[1]), points = cluster_centers)
```



```
[20]: # X_cl = X[y_db!=-1,:]
# y_db_cl = y_db[y_db!=-1]
# silhouette = silhouette_samples(X_cl,y_db_cl)
# plot_silhouette(silhouette,y_db_cl)
silhouette = silhouette_samples(X,y_db)
plot_silhouette(silhouette,y_db)
```



### ml-05-association-rules

February 12, 2020

## 1 Association Rules

#### 1.1 Example with the Online Retail dataset, from UCI

Code provided in this link

```
[1]: import pandas as pd from mlxtend.frequent_patterns import apriori from mlxtend.frequent_patterns import association_rules
```

Upload the file 'Online-Retail.xlsx'. It is a MS Excel file, you can read it with the Pandas' function read\_excel.

Inspect its content. It is a transactional database where the role of transaction identifier is played by the column InvoiceNo and the items are in the column Description.

The database has some problems: 1. some descriptions represent the same item but have different leading or trailing spaces, therefore they must be made uniform with the Pandas' function str.strip()

```
[2]: # url = 'http://archive.ics.uci.edu/ml/machine-learning-databases/00352/

→ Online%20Retail.xlsx'

# url = 'machineLearning-05-association-rules-lab/Online-Retail.xlsx'

# url = 'Online-Retail.xlsx'

# df0 = pd.read_excel(url)

url = 'Online-Retail.csv'

df0 = pd.read_csv(url)

df0.head(20)
```

```
[2]:
        InvoiceNo StockCode
                                                        Description
                                                                     Quantity
                                                                                \
           536365
                      85123A
                               WHITE HANGING HEART T-LIGHT HOLDER
     0
                                                                             6
     1
           536365
                       71053
                                               WHITE METAL LANTERN
                                                                             6
     2
           536365
                      84406B
                                    CREAM CUPID HEARTS COAT HANGER
                                                                             8
     3
           536365
                      84029G
                              KNITTED UNION FLAG HOT WATER BOTTLE
                                                                             6
     4
           536365
                      84029E
                                    RED WOOLLY HOTTIE WHITE HEART.
                                                                             6
     5
                       22752
                                      SET 7 BABUSHKA NESTING BOXES
                                                                             2
           536365
     6
           536365
                       21730
                                GLASS STAR FROSTED T-LIGHT HOLDER
                                                                             6
     7
                       22633
                                            HAND WARMER UNION JACK
                                                                             6
           536366
     8
                                         HAND WARMER RED POLKA DOT
                                                                             6
           536366
                       22632
```

```
9
              NaN
                       84879
                                    ASSORTED COLOUR BIRD ORNAMENT
                                                                           32
     10
           536367
                       22745
                                       POPPY'S PLAYHOUSE BEDROOM
                                                                            6
                                                                            6
     11
           536367
                       22748
                                        POPPY'S PLAYHOUSE KITCHEN
                                                                            8
     12
           536367
                       22749
                                FELTCRAFT PRINCESS CHARLOTTE DOLL
     13
           536367
                       22310
                                          IVORY KNITTED MUG COSY
                                                                            6
                       84969
                               BOX OF 6 ASSORTED COLOUR TEASPOONS
                                                                            6
     14
           536367
     15
                       22623
                                    BOX OF VINTAGE JIGSAW BLOCKS
                                                                            3
           536367
                                   BOX OF VINTAGE ALPHABET BLOCKS
                                                                            2
     16
           536367
                       22622
                                                                            3
     17
                                         HOME BUILDING BLOCK WORD
           536367
                       21754
     18
           536367
                       21755
                                         LOVE BUILDING BLOCK WORD
                                                                            3
     19
           536367
                       21777
                                      RECIPE BOX WITH METAL HEART
                                                                            4
                 InvoiceDate
                              UnitPrice
                                          CustomerID
                                                              Country
     0
         2010-12-01 08:26:00
                                    2.55
                                              17850.0
                                                       United Kingdom
         2010-12-01 08:26:00
                                    3.39
     1
                                              17850.0
                                                       United Kingdom
                                    2.75
     2
         2010-12-01 08:26:00
                                              17850.0
                                                       United Kingdom
                                    3.39
     3
         2010-12-01 08:26:00
                                              17850.0
                                                       United Kingdom
     4
         2010-12-01 08:26:00
                                    3.39
                                                       United Kingdom
                                              17850.0
                                    7.65
         2010-12-01 08:26:00
                                              17850.0
                                                       United Kingdom
     6
         2010-12-01 08:26:00
                                    4.25
                                              17850.0
                                                       United Kingdom
     7
         2010-12-01 08:28:00
                                    1.85
                                                       United Kingdom
                                              17850.0
     8
         2010-12-01 08:28:00
                                    1.85
                                              17850.0 United Kingdom
     9
         2010-12-01 08:34:00
                                    1.69
                                              13047.0 United Kingdom
     10
         2010-12-01 08:34:00
                                    2.10
                                              13047.0 United Kingdom
     11
         2010-12-01 08:34:00
                                    2.10
                                              13047.0 United Kingdom
     12
         2010-12-01 08:34:00
                                    3.75
                                              13047.0 United Kingdom
         2010-12-01 08:34:00
                                              13047.0 United Kingdom
     13
                                    1.65
         2010-12-01 08:34:00
                                    4.25
                                              13047.0 United Kingdom
     15
         2010-12-01 08:34:00
                                    4.95
                                              13047.0 United Kingdom
         2010-12-01 08:34:00
                                    9.95
                                              13047.0 United Kingdom
     16
     17
         2010-12-01 08:34:00
                                    5.95
                                              13047.0
                                                       United Kingdom
         2010-12-01 08:34:00
                                    5.95
     18
                                              13047.0
                                                       United Kingdom
     19
         2010-12-01 08:34:00
                                    7.95
                                              13047.0
                                                       United Kingdom
[3]: url_csv = 'Online-Retail.csv'
     df0.to_csv(url_csv, index=False)
[4]: df0.head()
[4]:
       InvoiceNo StockCode
                                                      Description
                                                                   Quantity
                                                                              \
          536365
                    85123A
                              WHITE HANGING HEART T-LIGHT HOLDER
                                                                           6
                                                                           6
     1
          536365
                     71053
                                             WHITE METAL LANTERN
     2
          536365
                    84406B
                                  CREAM CUPID HEARTS COAT HANGER
                                                                           8
     3
          536365
                    84029G
                             KNITTED UNION FLAG HOT WATER BOTTLE
                                                                           6
                                  RED WOOLLY HOTTIE WHITE HEART.
     4
          536365
                    84029E
                                                                           6
```

```
0 2010-12-01 08:26:00
                            2.55
                                     17850.0 United Kingdom
1 2010-12-01 08:26:00
                            3.39
                                     17850.0 United Kingdom
2 2010-12-01 08:26:00
                            2.75
                                     17850.0
                                             United Kingdom
3 2010-12-01 08:26:00
                            3.39
                                     17850.0 United Kingdom
4 2010-12-01 08:26:00
                            3.39
                                     17850.0
                                             United Kingdom
```

[5]: print("The number of unique Description values in the input file is {}".

→format(len(df0['Description'].unique())))

The number of unique Description values in the input file is 4224

```
[6]: df1 = df0
df1['Description'] = df0['Description'].str.strip()
```

[7]: print("After cleaning, the number of unique Description values in the input

→file is {}".format(len(df1['Description'].unique())))

After cleaning, the number of unique Description values in the input file is 4212

Some rows may not have an InvoiceNo and must be removed, because they cannot be used.

Check if there are such that rows and in case remove them. You can check with the Pandas' function isna and remove with dropna on axis=0, with the option subset

```
[8]: print("Rows with missing InvoiceNo before removing")
df1[df1['InvoiceNo'].isna()]
```

Rows with missing InvoiceNo before removing

[8]: InvoiceNo StockCode Description Quantity \
9 NaN 84879 ASSORTED COLOUR BIRD ORNAMENT 32

```
InvoiceDate UnitPrice CustomerID Country 9 2010-12-01 08:34:00 1.69 13047.0 United Kingdom
```

```
[9]: df2 = df1.dropna(axis=0, subset=['InvoiceNo'])
```

```
[10]: print("Rows with missing InvoiceNo after removing")
df2[df2['InvoiceNo'].isna()]
```

Rows with missing InvoiceNo after removing

[10]: Empty DataFrame

Columns: [InvoiceNo, StockCode, Description, Quantity, InvoiceDate, UnitPrice, CustomerID, Country]

Index: []

Some InvoiceNo start with a C. They are "credit transactions" and must be removed.

Check the number of rows containing C in InvoiceNo and remove them. At the moment the column InvoiceNo is a generic object, in order to be able to use string functions, such as contains, it must be transformed into str with astype.

```
[11]: print("There are {} rows containing 'C' in 'InvoiceNo'"
            .format(sum(df2['InvoiceNo'].astype('str').str.contains('C'))))
```

There are 9288 rows containing 'C' in 'InvoiceNo'

```
[12]: df3 = df2[~df2['InvoiceNo'].astype('str').str.contains('C')]
```

```
[13]: print("After removal, there are {} rows containing 'C' in 'InvoiceNo'"
            .format(sum(df3['InvoiceNo'].astype('str').str.contains('C'))))
```

After removal, there are 0 rows containing 'C' in 'InvoiceNo'

Several transactions include the item 'POSTAGE', which represents the mailing expenses. In this analysis we are not interested in it, therefore the rows with 'POSTAGE' will be removed.

```
[14]: container = 'Description'
     target = 'POSTAGE'
     print("There are {} rows containing {} in {}"\
           .format(sum(df2[container].astype('str').str.contains(target)), target,
```

There are 1961 rows containing POSTAGE in Description

```
[15]: df = df3[~df3[container].astype('str').str.contains(target)]
```

[16]: df.describe

```
[16]: <bound method NDFrame.describe of
                                                InvoiceNo StockCode
      Description Quantity \
                                    WHITE HANGING HEART T-LIGHT HOLDER
      0
                536365
                          85123A
                                                                                6
                536365
                           71053
                                                   WHITE METAL LANTERN
      1
                                                                                6
      2
                536365
                          84406B
                                        CREAM CUPID HEARTS COAT HANGER
                                                                                8
      3
                                  KNITTED UNION FLAG HOT WATER BOTTLE
                536365
                          84029G
                                                                                6
                536365
                          84029E
                                        RED WOOLLY HOTTIE WHITE HEART.
                                                                                6
                           22613
      541904
                581587
                                           PACK OF 20 SPACEBOY NAPKINS
                                                                               12
      541905
                           22899
                                           CHILDREN'S APRON DOLLY GIRL
                581587
                                                                                6
      541906
                581587
                           23254
                                          CHILDRENS CUTLERY DOLLY GIRL
                                                                                4
                                       CHILDRENS CUTLERY CIRCUS PARADE
      541907
                581587
                           23255
                                                                                4
      541908
                                          BAKING SET 9 PIECE RETROSPOT
                581587
                           22138
                                                                                3
                      InvoiceDate UnitPrice CustomerID
                                                                  Country
      0
              2010-12-01 08:26:00
                                         2.55
                                                  17850.0 United Kingdom
                                                  17850.0 United Kingdom
              2010-12-01 08:26:00
                                         3.39
      1
      2
              2010-12-01 08:26:00
                                         2.75
                                                  17850.0 United Kingdom
```

```
3
        2010-12-01 08:26:00
                                  3.39
                                            17850.0
                                                     United Kingdom
4
                                  3.39
        2010-12-01 08:26:00
                                            17850.0
                                                     United Kingdom
541904
        2011-12-09 12:50:00
                                  0.85
                                            12680.0
                                                             France
541905 2011-12-09 12:50:00
                                  2.10
                                            12680.0
                                                             France
541906 2011-12-09 12:50:00
                                  4.15
                                            12680.0
                                                             France
       2011-12-09 12:50:00
                                  4.15
541907
                                            12680.0
                                                             France
541908 2011-12-09 12:50:00
                                  4.95
                                            12680.0
                                                             France
```

[530786 rows x 8 columns]>

After the cleanup, we need to consolidate the items into 1 transaction per row with each product 1 hot encoded. For the sake of keeping the data set small, we are only looking at sales for France. However, in additional code below, we will compare these results to sales from Germany. Further country comparisons would be interesting to investigate.

Actions: 1. filter the rows 'Country='France'2. group by ['InvoiceNo', 'Description'] computing a sum on ['Quantity'] 3. use the unstack function to move the items from rows to columns 4. reset the index 5. fill the missing with zero (fillna(0)) 6. store the result in the new dataframe basket' and inspect it

[17]: Description	10 COLOUR SPACEBOY PEN	12 COLOURED PARTY BALLOONS	\
InvoiceNo			
536370	0.0	0.0	
536852	0.0	0.0	
536974	0.0	0.0	
537065	0.0	0.0	
537463	0.0	0.0	

```
Description 12 EGG HOUSE PAINTED WOOD 12 MESSAGE CARDS WITH ENVELOPES
InvoiceNo
536370
                                    0.0
                                                                       0.0
536852
                                    0.0
                                                                       0.0
536974
                                    0.0
                                                                       0.0
537065
                                    0.0
                                                                       0.0
537463
                                                                       0.0
                                    0.0
```

537065 537463		0.0	
Description InvoiceNo	12 PENCILS SMALL TUBE RED R	ETROSPOT 12 PENCILS S	MALL TUBE SKULL \
536370		0.0	0.0
536852		0.0	0.0
536974		0.0	0.0
537065		0.0	0.0
537463		0.0	0.0
Description InvoiceNo	12 PENCILS TALL TUBE POSY	12 PENCILS TALL TUBE F	RED RETROSPOT \
536370	0.0		0.0
536852	0.0		0.0
536974	0.0		0.0
537065	0.0		0.0
537463	0.0		0.0
Description InvoiceNo	12 PENCILS TALL TUBE WOODLA	ND WRAP VINTAGE PE	TALS DESIGN \
536370	0	.0	0.0
536852	0	.0	0.0
536974	0	.0	0.0
537065		.0	0.0
537463	0	.0	0.0
Description InvoiceNo	YELLOW COAT RACK PARIS FASH	ION YELLOW GIANT GARD	DEN THERMOMETER \
536370		0.0	0.0
536852		0.0	0.0
536974		0.0	0.0
537065		0.0	0.0
537463		0.0	0.0
Description InvoiceNo	YELLOW SHARK HELICOPTER ZI	NC STAR T-LIGHT HOLDE	ER \
536370	0.0	0.	0
536852	0.0	0.	
536974	0.0	0.	0
537065	0.0	0.	0
537463	0.0	0.	0
Description InvoiceNo	ZINC FOLKART SLEIGH BELLS	ZINC HERB GARDEN CONTA	INER \
536370	0.0		0.0
536852	0.0		0.0

536974 537065	0.0 0.0	0.0	
537463	0.0	0.0	
Description InvoiceNo	ZINC METAL HEART DECORATION ZINC T-LIGHT HOLDER	STAR LARGE	\
536370	0.0	0.0	
536852	0.0	0.0	
536974	0.0	0.0	
537065	0.0	0.0	
537463	0.0	0.0	
Description InvoiceNo	ZINC T-LIGHT HOLDER STARS SMALL		
536370	0.0		
536852	0.0		
536974	0.0		
537065	0.0		
537463	0.0		

[5 rows x 1562 columns]

There are a lot of zeros in the data but we also need to make sure any positive values are converted to a 1 and anything less the 0 is set to 0.

You can define a function encode\_units which takes a number and returns 0 if the number is 0 or less, 1 if the number is 1 or more. The function can be applied to basket with the Pandas' function applymap, the result is stored in the variable basket\_sets

This step will complete the one hot encoding of the data.

```
[18]: import matplotlib.pyplot as plt
%matplotlib inline
def encode_units(x):
    if x <= 0:
        return 0
    if x >= 1:
        return 1

basket_sets = basket.applymap(encode_units)
```

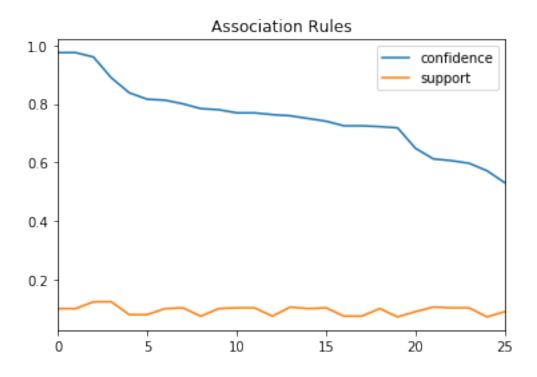
Now that the data is structured properly, we can generate frequent item sets that have a support of at least 7% (this number was chosen so that we can get enough useful examples):

- generate the frequent\_itemsets with apriori, setting min\_support=0.07 and use\_colnames=True
- generate the rules with association rules using metric="lift" and min\_threshold=1
- show the rules

```
[19]: frequent_itemsets = apriori(basket_sets, min_support=0.07, use_colnames=True)
      rules = association_rules(frequent_itemsets, metric="lift", min_threshold=1)
      rules.head()
[19]:
                          antecedents
                                                        consequents
         (ALARM CLOCK BAKELIKE GREEN)
                                        (ALARM CLOCK BAKELIKE PINK)
      1
          (ALARM CLOCK BAKELIKE PINK)
                                       (ALARM CLOCK BAKELIKE GREEN)
       (ALARM CLOCK BAKELIKE GREEN)
                                         (ALARM CLOCK BAKELIKE RED)
      2
      3
           (ALARM CLOCK BAKELIKE RED)
                                       (ALARM CLOCK BAKELIKE GREEN)
      4
           (ALARM CLOCK BAKELIKE RED)
                                        (ALARM CLOCK BAKELIKE PINK)
        antecedent support consequent support
                                                  support confidence
                                                                           lift \
                   0.098191
                                       0.103359 0.074935
      0
                                                             0.763158 7.383553
      1
                  0.103359
                                       0.098191 0.074935
                                                             0.725000 7.383553
      2
                  0.098191
                                       0.095607 0.080103
                                                             0.815789 8.532717
      3
                  0.095607
                                       0.098191 0.080103
                                                             0.837838 8.532717
                  0.095607
                                       0.103359 0.074935
                                                             0.783784 7.583108
        leverage
                  conviction
      0 0.064786
                     3.785817
      1 0.064786
                     3.279305
      2 0.070716
                     4.909561
      3 0.070716
                     5.561154
      4 0.065054
                     4.146964
```

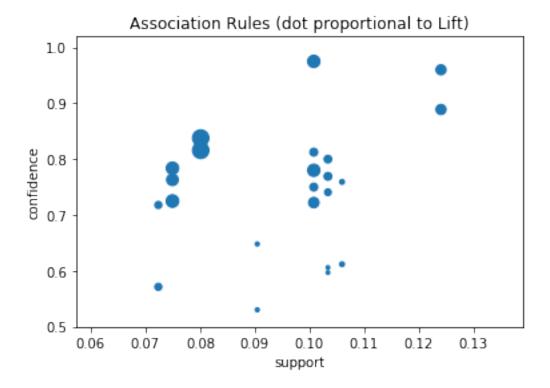
In order to plot the rules, it is better to sort them according to some metrics. We will sort on descending confidence and support and plot 'confidence' and 'support'.

[20]: <matplotlib.axes.\_subplots.AxesSubplot at 0x11eeaa610>



You find below a three dimensional plot, where the dot size is proportional to the lift, obtained using plot.scatter.

[21]: <matplotlib.axes.\_subplots.AxesSubplot at 0x11ef2c610>



Finally, we draw a plot of a subset of the rules using the function draw\_graph, provided in this package.

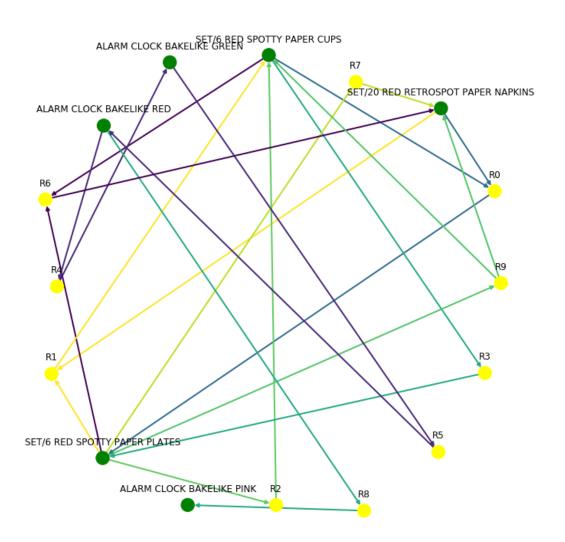
```
[23]: from draw_rules_graph import draw_graph help(draw_graph)
```

Help on function draw\_graph in module draw\_rules\_graph:

```
draw_graph(rules, rules_to_show=5)
   draws the rules as a graph linking antecedents and consequents
   "rule nodes" are yellow, with name "R<n>", "item nodes" are green
   arrows colors are different for each rule, and go from the antecedent(s)
   to the rule node and to the consequent(s)
   the "rules_to_show" parameter limits the rules to show to the initial
   part of the "rules" dataframe
```

```
[24]: import matplotlib.pyplot as plt
%matplotlib inline

plt.gcf().clear()
plt.figure(figsize=(10,10))
draw_graph (sorted_rules, 10)
```



[]:[

## ml-lab17-12-2019-dbscan

February 12, 2020

Claudio Sartori©

# 1 Machine Learning - Lab

## 1.1 Example of Lab exam

#### 1.1.1 Find the best clustering with DBSCAN

#### 2 Tasks

Find the clusters in the included dataset.

The solution must be produced as a Python Notebook. The notebook must include appropriate comments and must produce:

- 1. the boxplots of the attributes and a comment on remarkable situations, if any (2pt)
- 2. a pairplot of the data (see Seaborn pairplot) and a comment on remarkable situations, if any (2pt)
- 3. a clustering schema using a method of your choice exploring a range of parameter values (5pt)
- 4. the plot of the global inertia (SSD) and silhouette index for the parameter values you examine (4pt)
- 5. the optimal parameters of your choice (4pt)
- 6. a pairplot of the data using as hue the cluster assignment with the optimal parameter (3pt)
- 7. a plot of the silhouette index for the data points, grouped according to the clusters (4pt)
- 8. A sorted list of the discovered clusters for decreasing sizes (7pt)

NB: this solution is much more than what was requested for the exam

```
[1]: from IPython.display import Image
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd
from sklearn.cluster import DBSCAN
from sklearn.metrics import silhouette_score, silhouette_samples
from sklearn.preprocessing import MinMaxScaler
from sklearn.model_selection import ParameterGrid
```

```
from sklearn.preprocessing import MinMaxScaler

%matplotlib inline

rnd_state = 42 # This variable will be used in all the procedure calls allowing

a random_state parameter

# in this way the running can be perfectly reproduced

# just change this value for a different experiment

# the .py files with the functions provided must be in the same directory of

the .ipynb file

from plot_clusters import plot_clusters # python script provided separately

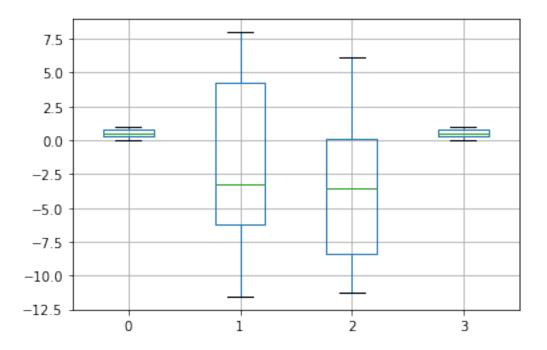
from plot_silhouette import plot_silhouette # python script provided separately
```

```
[2]: # data_file = 'ex1_4dim_data.csv'
# data_file = 'ex1_4dim_mod_data.csv'
# data_file = 'ex1_data.csv'
data_file = 'lab_exercise.csv'
delimiter = ','
X = np.loadtxt(data_file, delimiter = delimiter)
# scaler = MinMaxScaler()
# X = scaler.fit_transform(X)
```

- [3]: X.shape
- [3]: (1500, 4)

In order to exploit the Pandas DataFrame features we generate df from X

- [4]: df = pd.DataFrame(X)
  df.boxplot()
- [4]: <matplotlib.axes.\_subplots.AxesSubplot at 0x1084bea50>

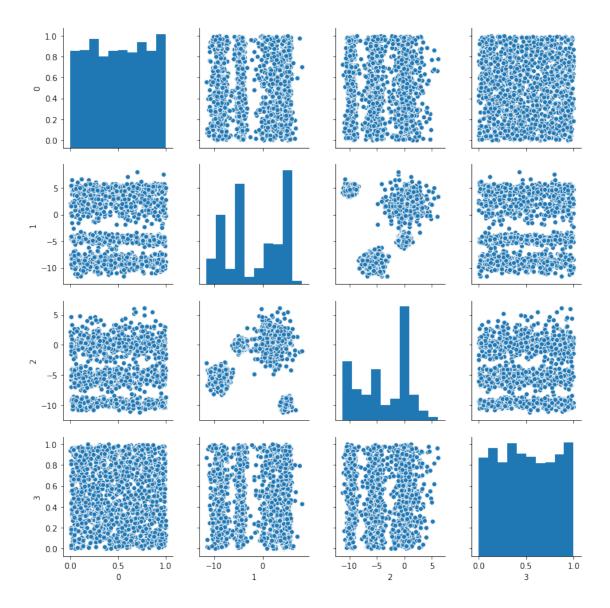


# 2.1 1. Comment on boxplots

Columns 0 and 3 have a range much smaller than 1 and 2. The distributions onf 0 and 3 seem to be equal. Poddibly, a min-max rescaling could point out some additional insight.

Let's look at the pairplots and consider if it is worth to do this transformation.

- [5]: sns.pairplot(pd.DataFrame(X))
- [5]: <seaborn.axisgrid.PairGrid at 0x1a1cd1fb50>



# 2.2 2. Comments on pairplots

The pairplots show that the two most interesting columns are 1 and 2, their pairplot shows evident clusters.

The pairplots of 0 and 3 show that those columns are uniformly distributed and do not show any pattern.

### 2.3 3. Find a clustering scheme with DBSCAN

We will try **k\_means** with a number of clusters varying from 2 to 10

Fit a DBSCAN estimator with the default parameters and examine the results.

```
[7]: db = DBSCAN()
y_db = db.fit_predict(X)
```

```
[8]: print(db)
```

DBSCAN(algorithm='auto', eps=0.5, leaf\_size=30, metric='euclidean', metric\_params=None, min\_samples=5, n\_jobs=None, p=None)

```
[9]: # Extract the unique labels
    cluster_labels_all = np.unique(y_db)
    # Exclude -1 (the label of noise) from the unique labels
    cluster_labels = cluster_labels_all[cluster_labels_all != -1]
    n_clusters = len(cluster_labels)
    # If there is noise the label -1 will be the first one,
    # according to the documentation
    if cluster_labels_all[0] == -1:
        noise = True
        print("There is noise")
    else:
        noise = False
    print("There is/are {} cluster(s)".format(n_clusters-noise))
```

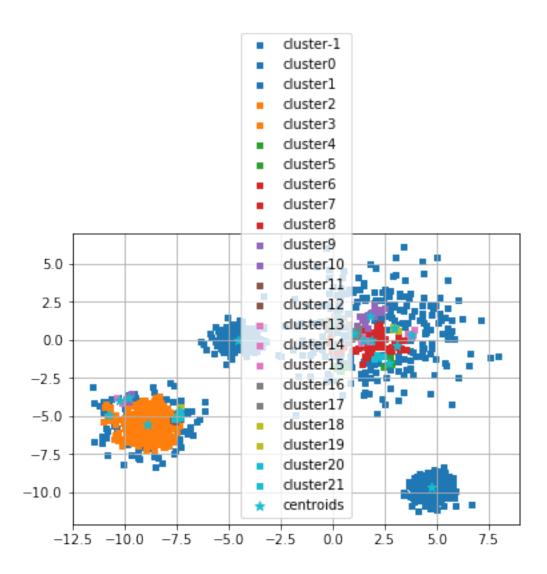
```
There is noise
There is/are 21 cluster(s)
```

Plot the clusters and their centers according to the clustering schema obtained with the default parameters. Plot only the dimensions which have been considered interesting.

```
[10]: # Prepare a data structure for the centroids
# the number of components is extracted from the shape of X
cluster_centers = np.empty((n_clusters, X.shape[1]))

# for each cluster label filter the data and compute the centroids
# as the mean along each component
for i in cluster_labels:
    cluster_centers[i,:] = np.mean(X[y_db==i,:], axis = 0)

# plot the clusters and the centroids
plot_clusters(X,y_db,dim=(int_cols[0],int_cols[1]), points = cluster_centers)
```



#### 2.3.1 Find the best parameters using ParameterGrid

```
# with silhouette above the threshold

clust_thr = 0.5 # visualize results only for combinations

# with ratio clustered/data above the threshold
```

```
[12]: def inertia_and_centers(X, y):
           ''' Computes the centroids and the inertia given a set of points X and \Box
       \hookrightarrow labels y
               Parameters:
                   : an array of shape[0] points in shape[1] dimensions
                   : a vector of labels corresponding to the points, proper labels
                      are in range 0...(shape[0]-1); possibly noise points are labelled<sub>□</sub>
       \hookrightarrow -1
               Uses the 'Einstein summation convention' from numpy for fast\sqcup
       \hookrightarrow computation of
               the inertia, see the [documentation](https://docs.scipy.org/doc/numpy/
       →reference/generated/numpy.einsum.html#numpy.einsum)
          cluster_labels_all = np.unique(y)
          cluster_labels = cluster_labels_all[cluster_labels_all != -1]
          n clusters = len(cluster labels)
          cluster_centers = np.empty((n_clusters, X.shape[1]))
          inertia = 0
          for i in cluster_labels:
               X_i = X[y==i,:]
               cluster_centers[i,:] = np.mean(X_i, axis = 0)
               X_i -= cluster_centers[i,:]
               inertia += np.einsum('ij,ij',X_i,X_i).mean()
          return inertia, cluster_centers, n_clusters
```

```
[13]: # Prepare a row to describe formatted output
      print("{:>11}\t{:>11}\t{:>11}\t{:>11}\t{:>11}\t{:>11}\.\
            format('eps','min_samp','n_clust','silh', 'clust_f', 'sc_index',_
      →'inertia'))
      # Prepare a dataframe for the results
      results = pd.DataFrame(columns=['eps', 'min_samp',
                                      'n_clust', 'silh', 'clust_f', 'sc_index', u
      →'inertia'l)
      # for each combination of parameter values executes clustering
      # then, saves the output if the quality measures are above the thresholds
      for i in range(len(params)):
          # initialise, then fit_predict the estimator, obtaining
         # the labelling; unclustered points (noise) are labelled -1
         db = DBSCAN(**(params[i]))
         y_db = db.fit_predict(X)
         # list of the proper cluster labels (excluding noise)
           cluster_labels_all = np.unique(y_db)
```

```
cluster_labels = cluster_labels_all[cluster_labels_all != -1]
inertia, cluster_centers, n_clusters = inertia_and_centers(X,y_db)
 n_clusters = len(cluster_labels)
# filters out the unclustered points
X_{cl} = X[y_{db}! = -1,:]
y_db_cl = y_db[y_db!=-1]
if n_clusters > 1 and n_clusters < X.shape[0]:</pre>
    # silhouette index cannot be computed out of this range
    silhouette = silhouette_score(X_cl,y_db_cl)
else:
    # 0 or N clusters
   silhouette = -2
clust = y_db_cl.shape[0]/y_db.shape[0] # fraction of clustered
# sc_index = an index computed as the armonic mean between
# Silhouette and the fraction of clustered
# (it is just a suggestion, it is not a standard measure, and
# it was not requested for the exercise)
sc_index = silhouette*clust/(silhouette+clust)
if silhouette > sil_thr and clust > clust_thr:
    # if above threshold save the results
   results = results.append({'eps':db.eps,
                              'min_samp':db.min_samples,
                              'n_clust':n_clusters,
                              'silh':silhouette,
                              'clust_f':clust,
                              'sc_index':sc_index,
                              'inertia':inertia,
                             },
                             ignore_index = True)
   print("{:11.2f}\t{:11}\t{:11}\t{:11.2f}\t{:11.2f}\t{:11.2f}\"\
          .format(db.eps, db.min_samples, n_clusters,
                  silhouette, clust, sc_index, inertia))
```

	eps	min_sa	mp	n_clust	silh	clust_f
sc_index		inertia				
	0.40		6	7	0.73	0.56
0.32		465.39				
	0.40		7	5	0.77	0.53
0.31		415.35				
	0.40		8	6	0.79	0.50
0.31		379.08				
	0.50		8	7	0.71	0.66
0.34		666.54				
	0.50		9	6	0.71	0.63
0.33		615.01				
	0.60		7	9	0.73	0.82
0.38		1151.12				

0.00	0.60	4004 05	8	7	0.76	0.79
0.39	0.60		9	7	0.78	0.76
0.39	0.70	1000.91	7	6	0.70	0.91
0.40	0.70	1966.82	8	6	0.71	0.90
0.40	0.80	1892.89	3	5	0.71	0.97
0.41	0.80	3004.98	4	4	0.76	0.96
0.42		2968.79				
0.42	0.80	2954.30	5	4	0.76	0.96
0.42	0.80	2641.71	8	4	0.77	0.94
0.42	0.80	2508.72	9	4	0.77	0.94
0.42	0.90	3214.11	3	4	0.75	0.97
0.42	0.90	3143.04	4	4	0.76	0.97
0.42	0.90		5	4	0.76	0.97
	0.90	3058.92	6	4	0.76	0.97
0.43	0.90		7	4	0.76	0.96
0.42	0.90	3003.08	8	4	0.76	0.96
0.43	0.90	2971.91	9	4	0.76	0.96
0.43	1.00	2921.37	5	4	0.75	0.97
0.42	1.00	3189.40	6	4	0.76	0.97
0.42	1.00	3113.40	7	4	0.76	0.97
0.42	1.00	3113.40	8	4	0.76	0.97
0.42		3113.40				
0.43	1.00	3063.74	9	4	0.76	0.97
0.42	1.10	3517.21	4	4	0.75	0.99
0.42	1.10	3459.19	5	4	0.75	0.98
0.43	1.10	3318.16	6	4	0.75	0.98

	1.10		7	4	0.75	0.98
0.43		3268.05				
	1.10		8	4	0.75	0.98
0.43		3241.27				
	1.10		9	4	0.75	0.98
0.43		3241.27				
	1.20		7	4	0.75	0.98
0.42		3450.50				
	1.20		8	4	0.75	0.98
0.42		3423.50				
	1.20		9	4	0.75	0.98
0.43		3353.96				
	1.30		9	4	0.75	0.99
0.42		3500.42				

#### 2.4 4. Plot of the inertia and silhouette

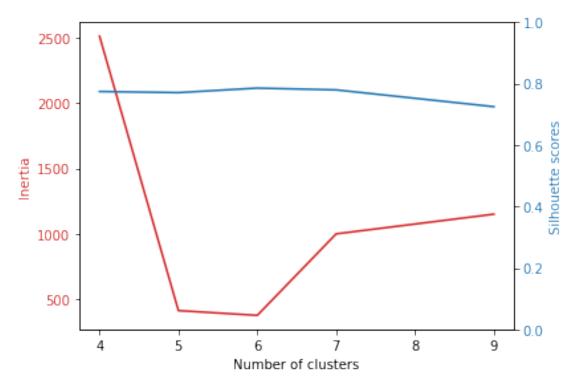
With DBSCAN the number of clusters is a dependent variable, being the independent ones eps and min\_samples. For this plot we will find, for each number of clusters, the combination of independent variables guaranteing the best silhouette index, using the thresholds filtered combinations stored in results.

The plot will not consider the noise points, otherwise the results would be obviously misleading.

```
[14]: # for each resulting number of clusters find the results row
# for which the silhouette index is maximum
idx_max_silh = results.groupby(['n_clust'])['silh'].transform(max) ==
□ → results['silh']
```

```
[15]: top_results = results[idx_max_silh].sort_values('n_clust')
```

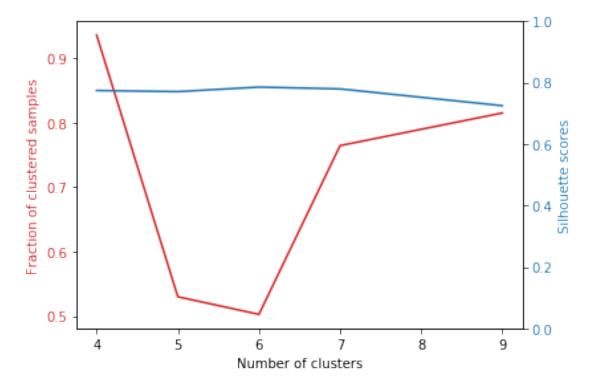
```
ax2.set_ylim(0,1) # the axis for silhouette is [0,1]
fig.tight_layout() # otherwise the right y-label is slightly clipped
plt.show()
```



For DBSCAN the *inertia* can be misleading, since it is naturally decreased for increasing number of *noise* samples. The *fraction of clustered samples* is probably more interesting in this case.

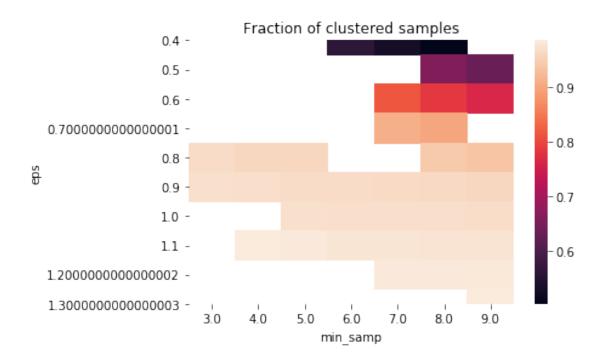
```
ax2.tick_params(axis='y', labelcolor=color)
ax2.set_ylim(0,1) # the axis for silhouette is [0,1]

fig.tight_layout() # otherwise the right y-label is slightly clipped
plt.show()
```

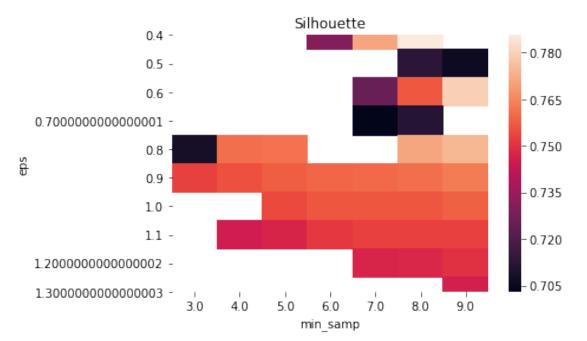


Additional insights can be obtained by the **heatmaps**, which allow to observe the results of pairs of parameters.

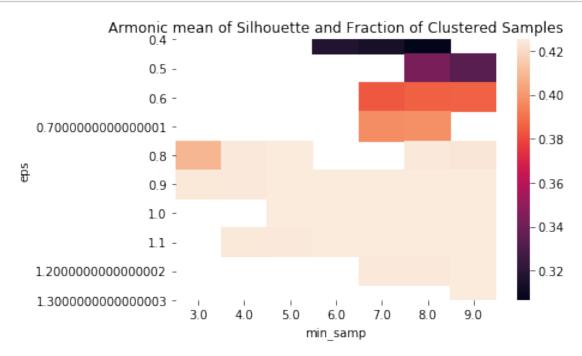
```
[18]: results_pivot =results.pivot('eps', 'min_samp', 'clust_f')
plt.title("Fraction of clustered samples")
ax = sns.heatmap(results_pivot)
```







```
[20]: results_pivot =results.pivot('eps', 'min_samp', 'sc_index')
plt.title("Armonic mean of Silhouette and Fraction of Clustered Samples")
ax = sns.heatmap(results_pivot)
```



#### 2.5 5. Show the best value for the parameter(s)

```
[21]: # find the row with the best results according to
# sc_index
best = results.iloc[results.index.argmax()]
```

```
[22]: print("Best tradeoff between Silhouette and Fraction of Clustered")
print("EPS = {:3.2f}\tMIN_SAMPLES = {:2.0f}".format(best.eps, best.min_samp))
print("Results with best parameters")
print("Silhouette = {:3.2f}\tClustered Fraction = {:3.2f}\tNumber of Clusters = 
→ {:2.0f}".\
format(best.silh, best.clust_f,best.n_clust))
```

```
Best tradeoff between Silhouette and Fraction of Clustered 

EPS = 1.30 MIN_SAMPLES = 9 Results with best parameters 

Silhouette = 0.75 Clustered Fraction = 0.99 Number of Clusters = 4
```

# 2.6 6. Cluster with the optimal parameter(s) and show the pairplot

```
[23]: db = DBSCAN(eps=best.eps, min_samples=int(best.min_samp))
      y_db = db.fit_predict(X)
[24]: df['cluster'] = y_db
      sns.pairplot(df[int_cols + ['cluster']], vars = df[int_cols], hue = 'cluster')
[25]:
[25]: <seaborn.axisgrid.PairGrid at 0x1a1d986850>
                  5
                  0
                -5
               -10
                                                                             duster
                                                                                  -1
                                                                                  0
                                                                                  1
                  5
                                                                                  2
                                                                                  3
                  0
               -10
                                       10
                      -10
                               0
                                                              0
                                                                      10
```

$$[26]: \# plot\_clusters(X, y\_db, dim=(int\_cols[0], int\_cols[1]), \ points = cluster\_centers)$$

### 2.7 7. Quantifying the quality of clustering via silhouette plots

1

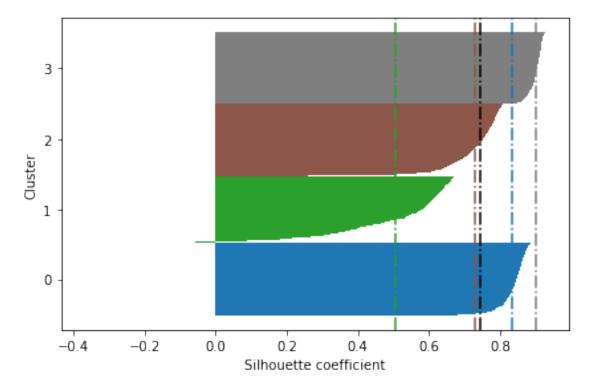
The silhouette scores for the individual samples are computed with the function  ${\tt silhouette\_samples}$ 

The function plot\_silhouette produces a 'horizontal bar-plot', with one bar for each sample, where the length of the bar is proportional to the silhouette score of the sample. The bars are grouped for cluster and sorted for decreasing length.

A vertical line represents the silhouette score, i.e. the average on all the samples.

```
[27]: # from plot_silhouette import plot_silhouette
from plot_silhouette2 import plot_silhouette
```

```
[28]: X_cl = X[y_db!=-1,:]
    y_db_cl = y_db[y_db!=-1]
    silhouette = silhouette_samples(X_cl,y_db_cl)
    plot_silhouette(silhouette,y_db_cl)
# silhouette = silhouette_samples(X,y_db)
# plot_silhouette(silhouette,y_db)
```



#### 2.8 8. Sorted list of the discovered clusters for decreasing sizes (7pt)

groupby().size() returns a dataframe, resetting the index we can name the newly created column with the counts

```
[29]: counts = pd.DataFrame(y_db).groupby(0).size().reset_index(name='Count')
print(counts)
```

```
0 Count
0 -1 20
1 0 378
2 1 352
3 2 375
4 3 375
```

```
[30]: counts = pd.DataFrame(y_db).groupby(0).size().reset_index(name='Count')
```

Then we rename the first column as Cluster, sort by descending values of the counts and print the dataframe without showing the index

```
Cluster Count
0 378
2 375
3 375
1 352
-1 20
```

### ml-lab17-12-2019-KMeans

February 12, 2020

Claudio Sartori©

## 1 Machine Learning - Lab

### 1.1 Example of Lab exam

#### 1.1.1 Find the best number of clusters with k means

#### 2 Tasks

Find the clusters in the included dataset.

The solution must be produced as a Python Notebook. The notebook must include appropriate comments and must produce:

- 1. the boxplots of the attributes and a comment on remarkable situations, if any (2pt)
- 2. a pairplot of the data (see Seaborn pairplot) and a comment on remarkable situations, if any (2pt)
- 3. a clustering schema using a method of your choice exploring a range of parameter values (5pt)
- 4. the plot of the global inertia (SSD) and silhouette index for the parameter values you examine (4pt)
- 5. the optimal parameters of your choice (4pt)
- 6. a pairplot of the data using as hue the cluster assignment with the optimal parameter (3pt)
- 7. a plot of the silhouette index for the data points, grouped according to the clusters (4pt)
- 8. A sorted list of the discovered clusters for decreasing sizes (7pt)

```
[1]: from IPython.display import Image import numpy as np import matplotlib.pyplot as plt import seaborn as sns import pandas as pd from sklearn.cluster import KMeans from sklearn.metrics import silhouette_score, silhouette_samples %matplotlib inline
```

```
rnd_state = 42 # This variable will be used in all the procedure calls allowing → a random_state parameter

# in this way the running can be perfectly reproduced

# just change this value for a different experiment
```

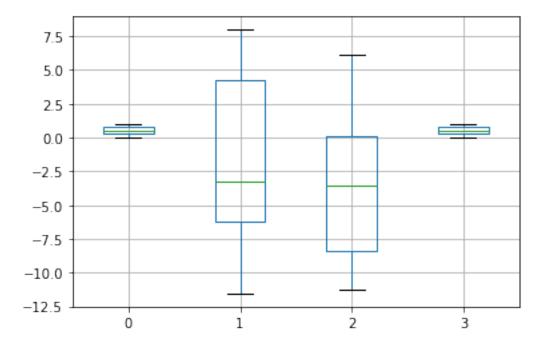
```
[2]: data_file = 'lab_exercise.csv'
delimiter = ','
X = np.loadtxt(data_file, delimiter = delimiter)
```

- [3]: X.shape
- [3]: (1500, 4)

In order to exploit the Pandas DataFrame features we generate df from X

```
[4]: df = pd.DataFrame(X)
df.boxplot()
```

[4]: <matplotlib.axes.\_subplots.AxesSubplot at 0x10ef8de90>



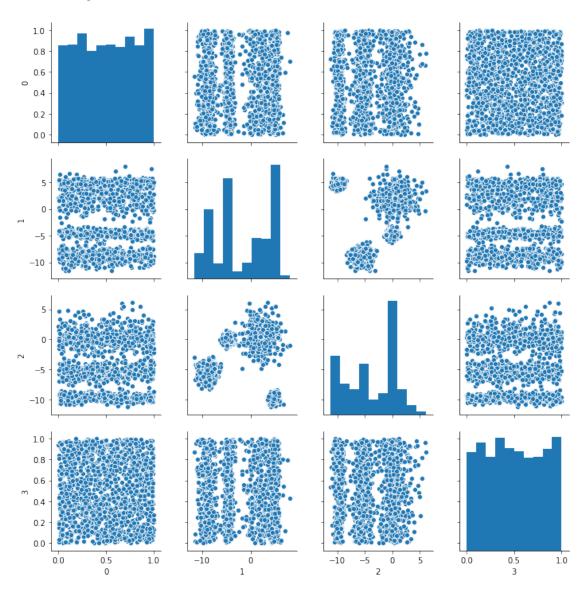
#### 2.1 1. Comment on boxplots

Columns 0 and 3 have a range much smaller than 1 and 2. The distributions onf 0 and 3 seem to be equal. Poddibly, a min-max rescaling could point out some additional insight.

Let's look at the pairplots and consider if it is worth to do this transformation.

## [5]: sns.pairplot(df)

## [5]: <seaborn.axisgrid.PairGrid at 0x1a236ded50>



## 2.2 2. Comments on pairplots

The pairplots show that the two most interesting columns are 1 and 2, their pairplot shows evident clusters.

The pairplots of 0 and 3 show that those columns are uniformly distributed and do not show any pattern.

```
[6]: int_cols = [1,2] # Interesting columns
```

#### 2.3 3. Find a clustering scheme with KMeans

We will try **k\_means** with a number of clusters varying from 2 to 10

- prepare two emptys lists for inertia and silhouette scores
- For each value of the number of clusters:
- initialize an estimator for KMeans and fit\_predict
- we will store the distortion (from the fitted model) in the variable distortions
- using the function silhouette\_score from sklearn.metrics with arguments the data and the fitted labels, we will fill the variable silhouette\_scores

Then we will plot the two lists in the y axis, with the range of k in the x axis. The plot with two different scales in the y axis can be done according to the example shown in the notebook two\_scales.ipynb.

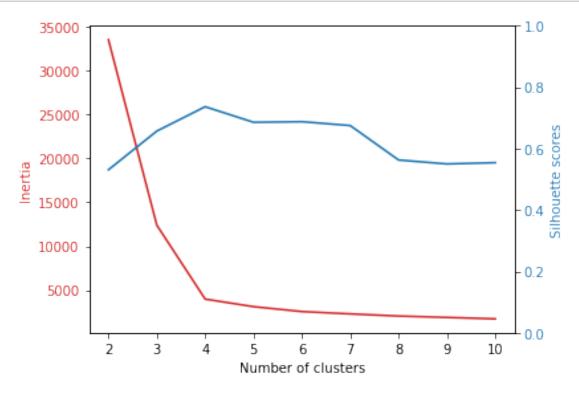
#### 2.4 4. Plot of inertia and silhouette

```
[9]: fig, ax1 = plt.subplots()

color = 'tab:red'
ax1.set_xlabel('Number of clusters')
ax1.set_ylabel('Inertia', color=color)
ax1.plot(k_range, distortions, color=color)
ax1.tick_params(axis='y', labelcolor=color)

ax2 = ax1.twinx() # instantiate a second axes that shares the same x-axis

color = 'tab:blue'
```



## 2.5 5. Show the best value for the parameter(s)

```
[10]: good_k = np.argmax(silhouette_scores) + k_range.start print("The value of K providing the maximum silhouette index is {}".

→format(good_k))
```

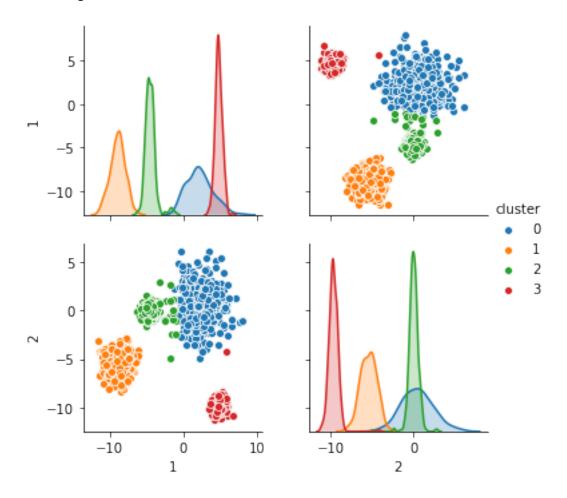
The value of K providing the maximum silhouette index is 4

## 2.6 6. Cluster with the optimal parameter(s) and show the pairplot

In order to show the "hue" with the Seaborn pairplot it is necessary to add the cluster column and then specify as vars the data columns you want to plot.

```
[12]: df['cluster'] = y_km
[13]: sns.pairplot(df[int_cols + ['cluster']], vars = df[int_cols], hue = 'cluster')
```

[13]: <seaborn.axisgrid.PairGrid at 0x1a240ae890>



#### 2.7 7. Quantifying the quality of clustering via silhouette plots

The silhouette scores for the individual samples are computed with the function silhouette\_samples

The function plot\_silhouette produces a 'horizontal bar-plot', with one bar for each sample, where the length of the bar is proportional to the silhouette score of the sample. The bars are grouped for cluster and sorted for decreasing length.

A vertical line represents the silhouette score, i.e. the average on all the samples

```
[14]: # from plot_silhouette import plot_silhouette
from plot_silhouette2 import plot_silhouette
```

```
[15]: help(plot_silhouette)
```

Help on function plot\_silhouette in module plot\_silhouette2:

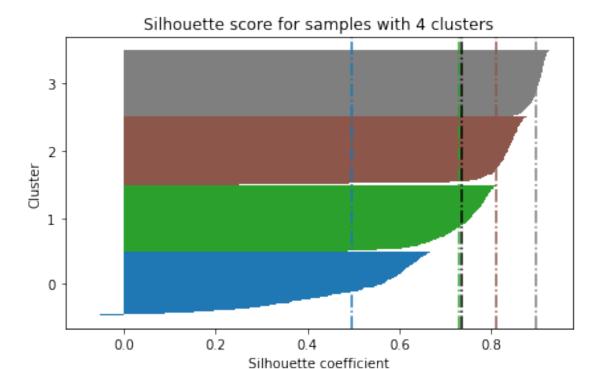
plot\_silhouette(silhouette\_vals, y, colors=<matplotlib.colors.ListedColormap
object at 0x11d48a0d0>, plot\_noise=False)

Plotting silhouette scores for the individual samples of a labelled data set.

The scores will be grouped according to labels and sorted in descending order.

The bars are proportional to the score and the color is determined by the label.

```
[16]: cluster_labels = np.unique(y_km)
    n_clusters = cluster_labels.shape[0] # it is the number of rows
# Compute the Silhouette Coefficient for each sample, with the euclidean metric
silhouette_score_samples = silhouette_samples(X, y_km, metric='euclidean')
plt.title('Silhouette score for samples with {} clusters'.format(good_k))
plot_silhouette(silhouette_score_samples, y_km)
```



### 2.8 8. Sorted list of the discovered clusters for decreasing sizes (7pt)

groupby().size() returns a dataframe, resetting the index we can name the newly created column with the counts

```
[17]: counts = pd.DataFrame(y_km).groupby(0).size().reset_index(name='Count')
print(counts)
```

- 0 Count
- 0 0 359
- 1 1 375
- 2 2 390
- 3 3 376

Then we rename the first column as Cluster, sort by descending values of the counts and print the dataframe without showing the index

- Cluster Count
  - 2 390
  - 3 376

- 1 375
- 0 359