





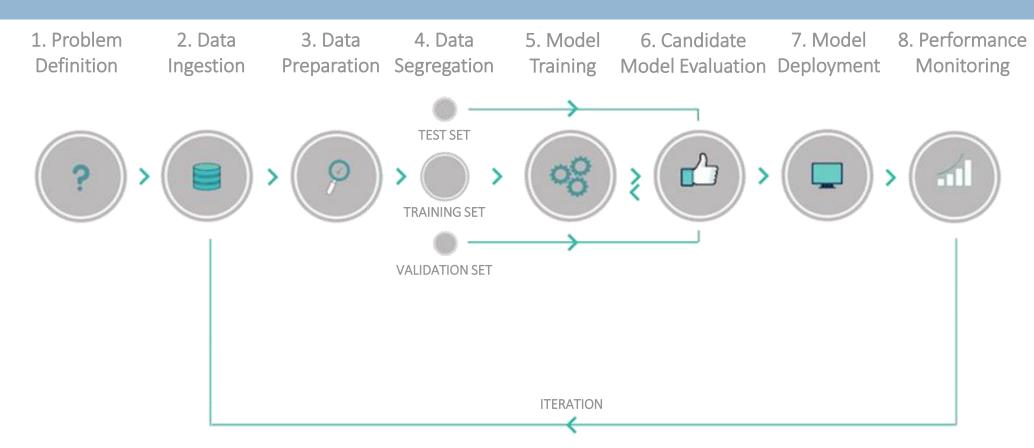
Dados e Aprendizagem Automática Data Exploration and Preparation

2

- Understanding the problem
- Data Exploration
- Data Preparation
- Hands On

https://semika.medium.com/

Understanding the problem



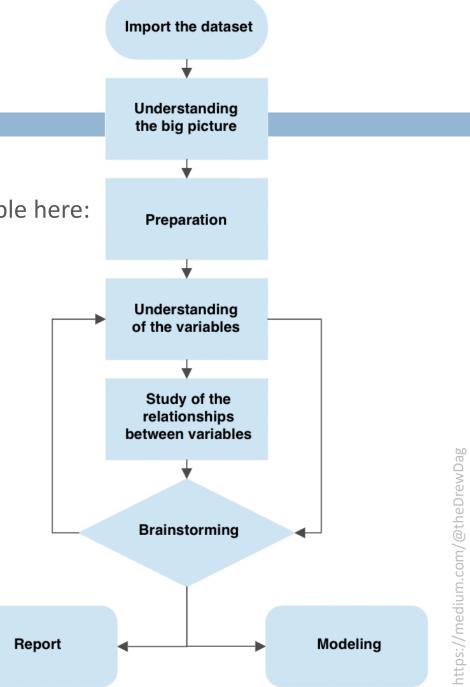
We must look to our data... We must understand it!

Data understanding is a huge step of the process and, as so, it will take its time! Nonetheless, it will give us a flavor of our dataset, at each variable, their meaning, and their relevance to this problem

4

Let's understand the features' type, how important it may be, if it is described in any other feature, ... Let's use the **wine dataset**, available here:

https://tinyurl.com/4cshpfac



Imports

Import libraries

```
import sklearn as skl
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn import preprocessing
```

Load the dataset and inspect some meta-data

```
Load CSV

df = pd.read_csv('wine.csv')
```

What about actual data? What can we see/get/understand from these data?

df.head()

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins	Color intensity	Hue	OD280/OD315 of diluted wines	Proline	Class
0	14.23	1.71	2.43	15.6	127	2.80	3.06	0.28	2.29	5.64	1.04	3.92	1065	one
1	13.20	1.78	2.14	11.2	100	2.65	2.76	0.26	1.28	4.38	1.05	3.40	1050	one
2	13.16	2.36	2.67	18.6	101	2.80	3.24	0.30	2.81	5.68	1.03	3.17	1185	one
3	14.37	1.95	2.50	16.8	113	3.85	3.49	0.24	2.18	7.80	0.86	3.45	1480	one
4	13.24	2.59	2.87	21.0	118	2.80	2.69	0.39	1.82	4.32	1.04	2.93	735	one

7

df.tail()

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins	Color intensity	Hue	OD280/OD315 of diluted wines	Proline	Class
173	13.71	5.65	2.45	20.5	95	1.68	0.61	0.52	1.06	7.7	0.64	1.74	740	three
174	13.40	3.91	2.48	23.0	102	1.80	0.75	0.43	1.41	7.3	0.70	1.56	750	three
175	13.27	4.28	2.26	20.0	120	1.59	0.69	0.43	1.35	10.2	0.59	1.56	835	three
176	13.17	2.59	2.37	20.0	120	1.65	0.68	0.53	1.46	9.3	0.60	1.62	840	three
177	14.13	4.10	2.74	24.5	96	2.05	0.76	0.56	1.35	9.2	0.61	1.60	560	three

df.shape

(178, 14)

We can see that we have 178 entries with 14 attributes each.

The Class has 3 classifications: one, two and three that refer to the type of wine.

```
#df.dtypes
df.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 178 entries, 0 to 177
Data columns (total 14 columns):
     Column
                                   Non-Null Count Dtype
     Alcohol
                                   178 non-null
                                                   float64
    Malic acid
                                   178 non-null
                                                   float64
     Ash
                                   178 non-null
                                                   float64
     Alcalinity of ash
                                   178 non-null
                                                   float64
    Magnesium
                                   178 non-null
                                                   int64
                                                   float64
    Total phenols
                                   178 non-null
     Flavanoids
                                   178 non-null
                                                   float64
     Nonflavanoid phenols
                                                   float64
                                   178 non-null
     Proanthocyanins
                                   178 non-null
                                                   float64
     Color intensity
                                                   float64
 9
                                   178 non-null
                                                   float64
 10
     Hue
                                   178 non-null
     OD280/OD315 of diluted wines 178 non-null
                                                   float64
     Proline
                                   178 non-null
                                                   int64
    Class
                                   178 non-null
                                                   object
dtypes: float64(11), int64(2), object(1)
memory usage: 19.6+ KB
```

There aren't null values and the attributes are all numeric except the Class.

9

We can also get some descriptive stats (for the entire numerical data or just the desired ones)...

df.describe()

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins	Color intensity	Hue	OD280/OD315 of diluted wines	Proline
count	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000	178.000000
mean	13.000618	2.336348	2.366517	19.494944	99.741573	2.295112	2.029270	0.361854	1.590899	5.058090	0.957449	2.611685	746.893258
std	0.811827	1.117146	0.274344	3.339564	14.282484	0.625851	0.998859	0.124453	0.572359	2.318286	0.228572	0.709990	314.907474
min	11.030000	0.740000	1.360000	10.600000	70.000000	0.980000	0.340000	0.130000	0.410000	1.280000	0.480000	1.270000	278.000000
25%	12.362500	1.602500	2.210000	17.200000	88.000000	1.742500	1.205000	0.270000	1.250000	3.220000	0.782500	1.937500	500.500000
50%	13.050000	1.865000	2.360000	19.500000	98.000000	2.355000	2.135000	0.340000	1.555000	4.690000	0.965000	2.780000	673.500000
75%	13.677500	3.082500	2.557500	21.500000	107.000000	2.800000	2.875000	0.437500	1.950000	6.200000	1.120000	3.170000	985.000000
max	14.830000	5.800000	3.230000	30.000000	162.000000	3.880000	5.080000	0.660000	3.580000	13.000000	1.710000	4.000000	1680.000000

df['Color intensity'].describe()

count 178.000000
mean 5.058090
std 2.318286
min 1.280000
25% 3.220000
50% 4.690000
75% 6.200000
max 13.000000

Name: Color intensity, dtype: float64

What about missing values?

```
Missing data

df.isna().any()
```

Alcohol False Malic acid False False Ash Alcalinity of ash False Magnesium False Total phenols False Flavanoids False Nonflavanoid phenols False Proanthocyanins False Color intensity False False Hue OD280/OD315 of diluted wines False Proline False Class False dtype: bool

print(df.isna().sum()) Alcohol 0 Malic acid Ash Alcalinity of ash Magnesium Total phenols Flavanoids Nonflavanoid phenols Proanthocyanins Color intensity Hue OD280/OD315 of diluted wines 0 Proline 0 Class 0 dtype: int64

With our analysis, we can characterize better the dataset:

- It has 178 entries
- 14 attributes 13 are physical-chemical properties of the wine and 1 is the classification
- All non-null values
- There aren't missing values

The **goal** of working with this dataset can be **identify the type of wine by its properties** - the target is a numeric categorical variable that covers the values of one, two and three.

If used for modeling, the features of the wine can be used to predict its type.

Data Preparation

It consists of multiple steps... Many times (in reality, a lot of times), you'll need to check the API of the lib you are using... Hera are some links you may save for future reference:

- Numpy (https://numpy.org/doc/stable/)
- Pandas (https://pandas.pydata.org/docs/)
- Matplotlib (<u>https://matplotlib.org/stable/contents.html</u>)
- Seaborn (https://seaborn.pydata.org/api.html)
- Scikit Learn (https://scikit-learn.org/stable/modules/classes.html)

Data Preparation

And here are some basic Pandas functions you'll need (somewhen) in the future for data prep.:

- pandas.DataFrame.drop
- pandas.DataFrame.drop_duplicates
- pandas.DataFrame.fillna
- pandas.DataFrame.isna
- pandas.DataFrame.interpolate
- pandas.DataFrame.dropna
- pandas.DataFrame.groupby
- pandas.DataFrame.loc
- pandas.DataFrame.iloc
- •

Data Preparation

And here are some basic sklearn functions/classes you'll need (somewhen) in the future for data prep.:

- sklearn.preprocessing.MinMaxScaler
- sklearn.preprocessing.StandardScaler
- sklearn.preprocessing.KBinsDiscretizer
- sklearn.preprocessing.LabelEncoder
- sklearn.feature_selection
- sklearn.metrics
- •

111

Data Preparation and Transformation

Remove duplicate values

```
Drop Duplicates
print(df.duplicated().sum())
print(df.drop_duplicates(inplace=True))
print(df.info())
0
None
<class 'pandas.core.frame.DataFrame'>
Int64Index: 178 entries, 0 to 177
Data columns (total 14 columns):
     Column
                                   Non-Null Count Dtvpe
     Alcohol
                                   178 non-null
                                                    float64
     Malic acid
                                   178 non-null
                                                    float64
     Ash
                                   178 non-null
                                                    float64
     Alcalinity of ash
                                   178 non-null
                                                    float64
     Magnesium
                                   178 non-null
                                                    int64
     Total phenols
                                   178 non-null
                                                    float64
     Flavanoids
                                   178 non-null
                                                    float64
     Nonflavanoid phenols
                                   178 non-null
                                                    float64
     Proanthocyanins
                                                    float64
                                   178 non-null
     Color intensity
                                   178 non-null
                                                    float64
                                                    float64
 10
     Hue
                                   178 non-null
     OD280/OD315 of diluted wines 178 non-null
                                                    float64
     Proline
                                   178 non-null
                                                    int64
 13 Class
                                   178 non-null
                                                   object
dtypes: float64(11), int64(2), object(1)
memory usage: 20.9+ KB
None
```

Rename attributes

```
1.1.1
Rename complicated columns' names
df.rename(columns={"OD280/OD315 of diluted wines": "Protein Concentration"}, inplace=True)
df.info()
<class 'pandas.core.frame.DataFrame'>
Int64Index: 178 entries, 0 to 177
Data columns (total 14 columns):
     Column
                            Non-Null Count Dtype
     Alcohol
                            178 non-null
                                             float64
    Malic acid
                            178 non-null
                                             float64
    Ash
                            178 non-null
                                             float64
    Alcalinity of ash
                            178 non-null
                                            float64
    Magnesium
                            178 non-null
                                             int64
    Total phenols
                            178 non-null
                                            float64
                            178 non-null
    Flavanoids
                                            float64
                            178 non-null
    Nonflavanoid phenols
                                             float64
    Proanthocyanins
                            178 non-null
                                             float64
                                            float64
    Color intensity
                            178 non-null
 10
    Hue
                            178 non-null
                                            float64
    Protein Concentration 178 non-null
                                            float64
    Proline
                            178 non-null
                                             int64
 13 Class
                                             object
                            178 non-null
dtypes: float64(11), int64(2), object(1)
memory usage: 20.9+ KB
```

Data Preparation and Transformation

```
111
Remove values (Ash smaller than 2, Alcalinity bigger than 15)
1.1.1
df_clean = df.drop(df.loc[(df['Ash']<2) & (df['Alcalinity of ash']>15)].index)
print(df_clean)
#df.drop(df.loc[(df['Ash']<2) & (df['Alcalinity of ash']>15)].index, inplace=True) ##alternative
                           Ash Alcalinity of ash Magnesium Total phenols \
     Alcohol Malic acid
      14.23
                    1.71 2.43
                                              15.6
                                                          127
                                                                         2.80
       13.20
                    1.78 2.14
                                              11.2
                                                          100
                                                                         2.65
      13.16
                    2.36 2.67
                                              18.6
                                                          101
                                                                         2.80
      14.37
                    1.95 2.50
3
                                              16.8
                                                          113
                                                                         3.85
      13.24
                    2.59 2.87
                                              21.0
                                                          118
                                                                        2.80
       13.71
                    5.65 2.45
                                              20.5
173
                                                           95
                                                                        1.68
174
       13.40
                    3.91 2.48
                                              23.0
                                                          102
                                                                        1.80
175
       13.27
                    4.28 2.26
                                              20.0
                                                                        1.59
                                                          120
176
       13.17
                    2.59 2.37
                                              20.0
                                                          120
                                                                         1.65
177
       14.13
                    4.10 2.74
                                              24.5
                                                           96
                                                                        2.05
                 Nonflavanoid phenols
                                       Proanthocyanins
                                                         Color intensity
     Flavanoids
0
           3.06
                                  0.28
                                                   2.29
                                                                    5.64 1.04
1
           2.76
                                  0.26
                                                   1.28
                                                                    4.38 1.05
           3.24
                                  0.30
                                                   2.81
                                                                    5.68 1.03
3
           3.49
                                  0.24
                                                   2.18
                                                                    7.80
                                                                          0.86
           2.69
                                  0.39
                                                   1.82
                                                                    4.32 1.04
            . . .
                                   . . .
173
           0.61
                                  0.52
                                                   1.06
                                                                    7.70
                                                                          0.64
174
           0.75
                                  0.43
                                                   1.41
                                                                          0.70
                                                   1.35
175
           0.69
                                  0.43
                                                                    10.20
                                                                           0.59
176
           a es
                                  a 53
                                                   1 46
                                                                    0 30
                                                                          0 60
```

Since all the variables appear to be physical-chemical measures, they could all be useful and help define the segmentation of the type of wine. There is no reason to remove columns.

Univariate Analysis

Iterate through each and every relevant variable and get basic information.

```
1.1.1
Categorical variables
df['Alcohol'].value counts()
12.37
13.05
12.08
12.29
12.00
         3
13.34
13.69
13.90
13.84
         1
13.75
Name: Alcohol, Length: 126, dtype: int64
df['Class'].value_counts(normalize=True)
         0.398876
two
         0.331461
one
         0.269663
three
Name: Class, dtype: float64
```

```
1.1.1
Numeric variables
1.1.1
df['Magnesium'].describe()
         178.000000
count
          99.741573
mean
          14.282484
std
min
          70.000000
25%
          88.000000
50%
          98.000000
75%
         107.000000
         162.000000
max
Name: Magnesium, dtype: float64
```

Univariate Analysis

```
print(f"Histogram: {df['Magnesium'].hist()}")
Histogram: AxesSubplot(0.125,0.125;0.775x0.755)
40
30
20
10
                                      140
                   100
                            120
                                                160
```

Does not follow a normal curve and has spikes.

```
print(f"Skewness: {df['Magnesium'].skew()}")
Skewness: 1.098191054755161
```

```
print(f"Kurtosis: {df['Magnesium'].kurt()}")
```

Kurtosis: 2.1049913235905557

Kurtosis and asymmetry values are greater than 1.

Univariate Analysis

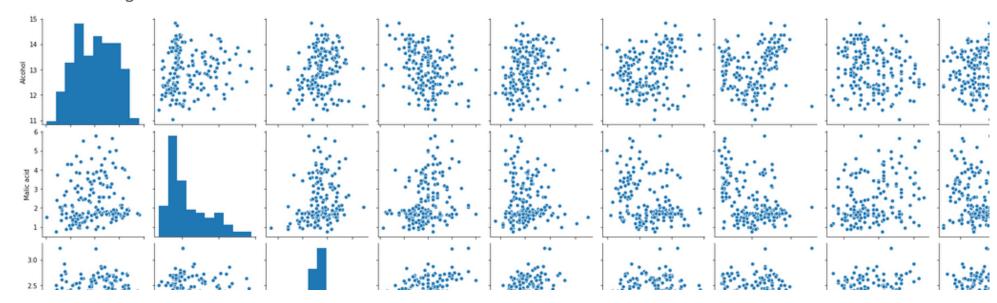
Now we can summarize the dataset creating a small document with detailed information:

- *Variable*: name of the variable
- Type: the type or format of the variable. This can be categorical, numeric, Boolean, and so on
- *Context*: useful information to understand the semantic space of the variable. In the case of our dataset, the context is always the chemical-physical one
- Expectation: how relevant is this variable with respect to our task? We can use a scale "High, Medium, Low".
- Comments: whether or not we have any comments to make on the variable

We can start by seeing the relation between all variables:

```
All variables
sns.pairplot(df)
```

<seaborn.axisgrid.PairGrid at 0x7f08ccac79d0>



. . .

We can group by variables:

```
Grouping
'''

df.groupby(by=['Class']).mean()
```

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Ρ.
Class									
one	13.744746	2.010678	2.455593	17.037288	106.338983	2.840169	2.982373	0.290000	
three	13.153750	3.333750	2.437083	21.416667	99.312500	1.678750	0.781458	0.447500	
two	12.278732	1.932676	2.244789	20.238028	94.549296	2.258873	2.080845	0.363662	

df.gr	oupby(b	y=['Clas	ss', 'Prol	ine'])	.mean()					
		Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	••
Class	Proline									
one	680	13.240	3.980	2.290	17.5	103.0	2.640	2.630	0.32	
	735	13.240	2.590	2.870	21.0	118.0	2.800	2.690	0.39	
	760	14.220	3.990	2.510	13.2	128.0	3.000	3.040	0.20	
	770	12.930	3.800	2.650	18.6	102.0	2.410	2.410	0.25	
	780	14.060	1.630	2.280	16.0	126.0	3.000	3.170	0.24	
two	750	12 835	0 965	2 155	15 9	123.0	2 215	1 575	0.45	

We can group by variables:

	Malic acid	Ash	Alcalinity of ash	Total phenols	\
Alcohol					
11.03	1.51	2.2	21.5	2.46	
11.41	0.74	2.5	21	2.48	
11.45	2.4	2.42	20	2.9	
11.46	3.74	1.82	19.5	3.18	
11.56	2.05	3.23	28.5	3.18	
L4.37	1.95	2.5	16.8	3.85	
L4.38	[1.87, 3.59]	[2.28, 2.38]	[12.0, 16.0]	[3.25, 3.3]	
L4.39	1.87	2.45	14.6	2.5	
L4.75	1.73	2.39	11.4	3.1	
14.83	1.64	2.17	14	2.8	
	Flavanoids	Nonflavanoid p	henols Proanthocya	anins Color int	ensity
Alcohol					
11.03	2.17		0.52	2.01	1.9
11.41	2.01		0.42	1.44	3.08
l1.45	2.79		0.32	1.83	3.25
11 10	2 50		0.34	י רט	2 0

11.03 2 11.41 2 11.45 2 11.46 2 11.56 5 14.38 3 14.39 2 14.75 3	Flavanoids 2.17 2.01 2.79 2.58 5.08 3.17	naire	1.51 0.74 2.40 3.74 2.05 	2.20 2.50 2.42 1.82 3.2	21.0 2 20.0 2 19.5 3 28.5	85 88 96 107 119	`
11.41 2 11.45 2 11.46 2 11.56 5 14.38 3 14.39 2 14.75 3	2.01 2.79 2.58 5.08 3.17		0.74 2.40 3.74 2.05 3.59	2.56 2.42 1.82 3.2	21.0 2 20.0 2 19.5 3 28.5	88 96 107 119	
11.45 2 11.46 2 11.56 5 14.38 3 14.39 2 14.75 3	2.79 2.58 5.08 3.17 3.64		2.40 3.74 2.05 3.59	2.42 1.82 3.2	2 20.0 2 19.5 3 28.5	96 107 119	
11.46 2 11.56 5 14.38 3 14.39 2 14.75 3	2.58 5.08 3.17 3.64		3.74 2.05 3.59	1.82 3.2	2 19.5 3 28.5	107 119	
11.56 5 14.38 3 14.39 2 14.75 3	3.17 3.64		2.05 3.59	3.2	3 28.5	119	
 14.38 3 3 14.39 2 14.75 3	3.17 3.64		3.59				
14.38 3 3 14.39 2 14.75 3	3.64		3.59				
3 14.39 2 14.75 3	3.64			2.28	2 16 A	102	
14.39 2 14.75 3					10.0	102	
14.75 3			1.87	2.38	3 12.0	102	
	2.52		1.87	2.45	14.6	96	
14.83 2	3.69		1.73	2.39	11.4	91	
	2.98		1.64	2.17	7 14.0	97	
		Total	pheno	ls N	Nonflavanoid phenols	Proanthocv	anins
Alcohol F	lavanoids		pe				
	2.17		2.	46	0.52		2.01
	2.01		2.		0.42		1.44
	2.79		2.		0.32		1.83
	2.58		3.		0.24		3.58
	5.08		3.		0.47		1.87
14.38 3	3.17		3.	25	0.27		2.19
3	3.64		3.	30	0.29		2.96

We can create bins.

Data binning (or bucketing) groups data in bins (or buckets), in the sense that it replaces values contained into a small interval with a single representative value for that interval. It is a type of data preprocessing, a mechanism which includes also dealing with missing values, formatting, normalization and standardization.

Binning is a technique for data smoothing. Data smoothing is employed to remove noise from data.

```
111
Bins
1.1.1
# https://scikit-learn.org/stable/modules/preprocessing.html#discretization
estimator = preprocessing.KBinsDiscretizer(n bins=3, encode='ordinal', strategy='quantile')
df['alcohol binned'] = estimator.fit transform(df[['Alcohol']])
print('Bin Edges')
print(estimator.bin edges [0])
print('Alcohol Groups')
print(df.groupby(by=['alcohol binned']).count())
Bin Edges
[11.03 12.52 13.48 14.83]
Alcohol Groups
                Alcohol Malic acid Ash Alcalinity of ash Magnesium \
alcohol_binned
                     59
                                      59
                                                                     59
0.0
                                                          59
1.0
                     58
                                 58
                                      58
                                                          58
                                                                     58
2.0
                     61
                                 61
                                      61
                                                          61
                                                                     61
                Total phenols Flavanoids Nonflavanoid phenols \
alcohol_binned
0.0
                           59
                                                              59
1.0
                           58
                                       58
                                                              58
2.0
                           61
                                       61
                                                              61
                Proanthocyanins Color intensity Hue Protein Concentration \
alcohol binned
0.0
                             59
                                                    59
                                                                           59
                             52
                                                                           52
```

. . .

Dispersion: does it follow a Gaussian distribution?

```
Statistical Dispersion

fig, axs = plt.subplots(2, 2, figsize=(12, 10))

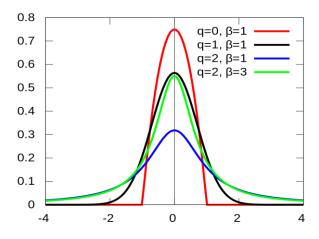
fig.suptitle('Histograms')

sns.distplot(df['Alcohol'], ax=axs[0, 0], kde=True)

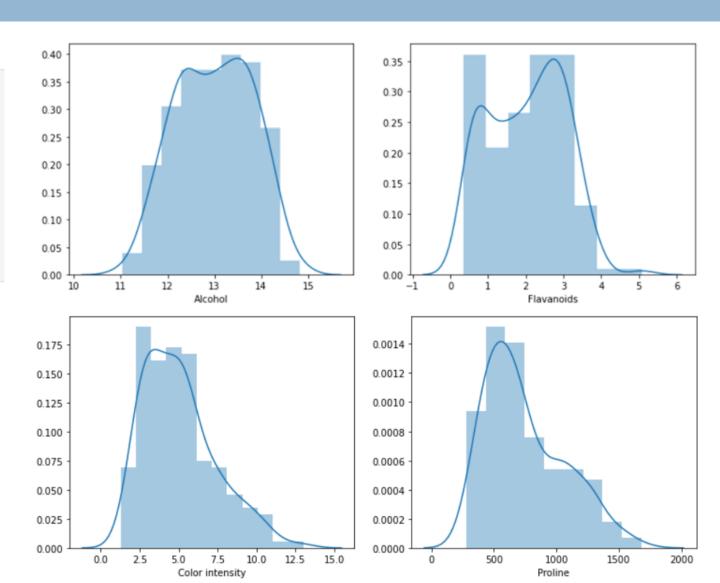
sns.distplot(df['Flavanoids'], ax=axs[0, 1], kde=True)

sns.distplot(df['Color intensity'], ax=axs[1, 0], kde=True)

sns.distplot(df['Proline'], ax=axs[1, 1], kde=True)
```



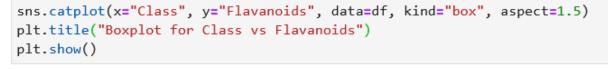
https://en.wikipedia.org/wiki/Q-Gaussian_distribution

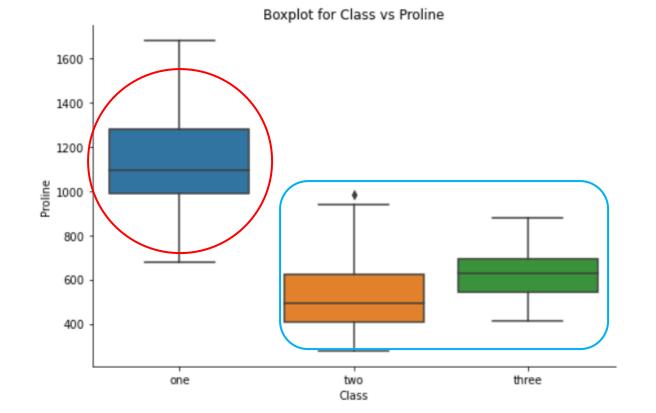


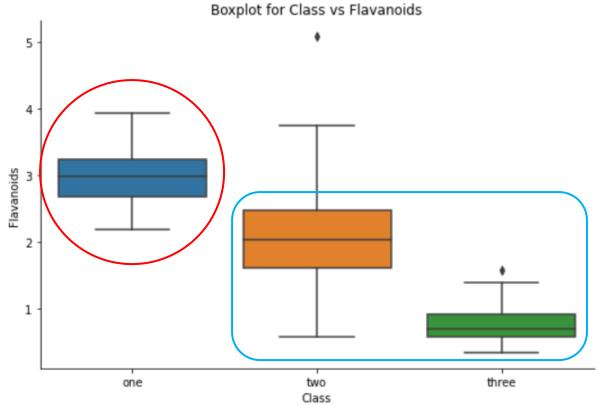
plt.show()

Multivariate Analysis

```
The best way to understand the relationship between a numeric variable and a categorical variable is
111
                      through a boxplot.
Box plots (Outliers)
sns.catplot(x="Class", y="Proline", data=df, kind="box", aspect=1.5)
plt.title("Boxplot for Class vs Proline")
```

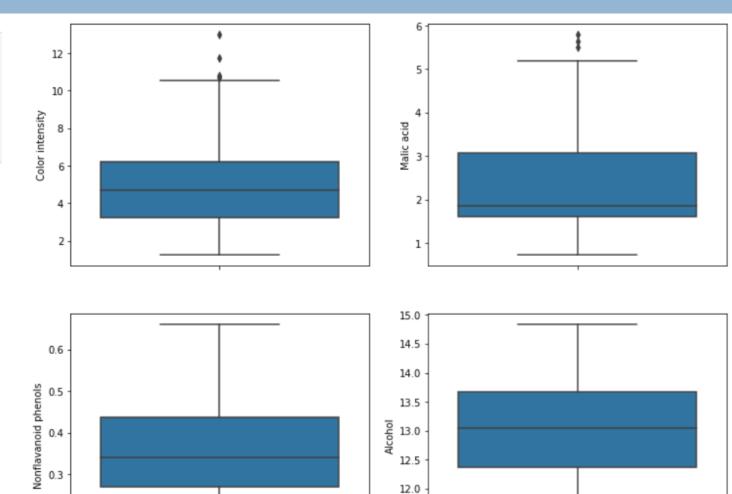






```
_, ax = plt.subplots(figsize=(15, 6))
fig.suptitle('Boxplot for Flavanoids vs Proline')
sns.boxplot(x=df["Flavanoids"], y=df["Proline"])
<AxesSubplot:xlabel='Flavanoids', ylabel='Proline'>
  1600
  1400
  1200
Proline
  1000
   800
   600
   400
                                                                 Flavanoids
```

```
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
fig.suptitle('Boxplots for 4 variables')
sns.boxplot(y=df['Color intensity'], ax=axs[0, 0])
sns.boxplot(y=df['Malic acid'], ax=axs[0, 1])
sns.boxplot(y=df['Nonflavanoid phenols'], ax=axs[1, 0])
sns.boxplot(y=df['Alcohol'], ax=axs[1, 1])
```



12.0

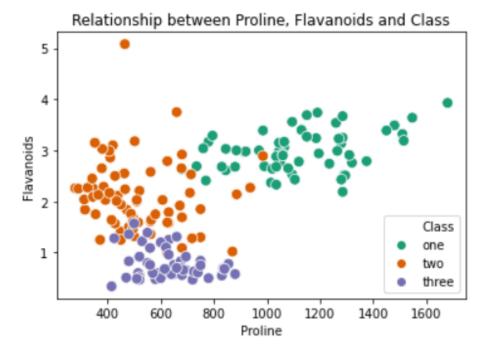
11.5

11.0

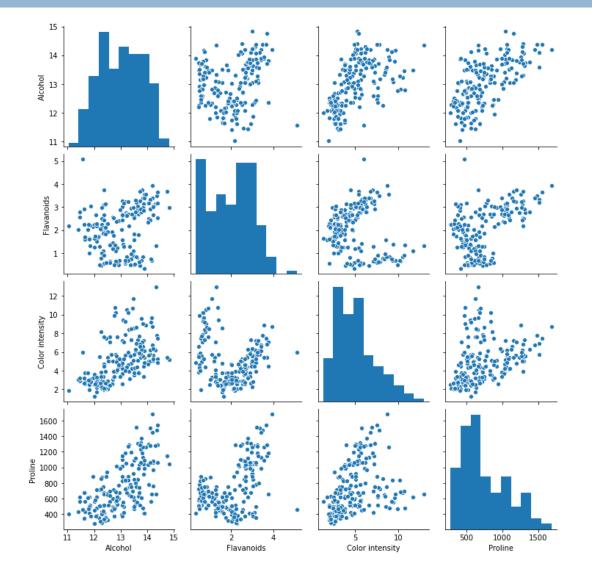
0.2

```
Scatter plots
""

sns.scatterplot(x="Proline", y="Flavanoids", hue="Class", data=df, palette="Dark2", s=80)
plt.title("Relationship between Proline, Flavanoids and Class")
plt.show()
```



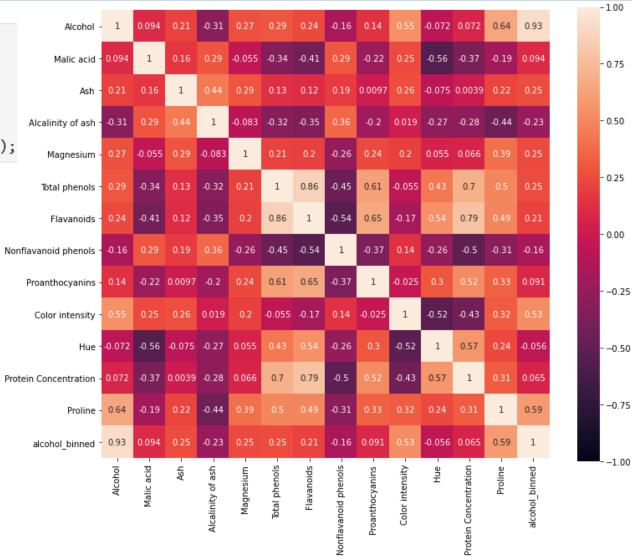
For class one the proline levels are much higher while the flavanoid level is stable around the value of 3.



```
Correlation
corr_matrix = df.corr()
f, ax = plt.subplots(figsize=(12, 10))
sns.heatmap(corr_matrix, vmin=-1, vmax=1, square=True, annot=True);
```

When the Class variable decreases (tendency to go to 0) the flavanoids, total phenols, proline and other proteins tend to increase. And viceversa.

There is a very strong correlation between alcohol and proline. High levels of alcohol correspond to high levels of proline.



Critical Analysis

Which components characterize the various types of wine?

Which component is the most significant?

. . .

Hands On

