





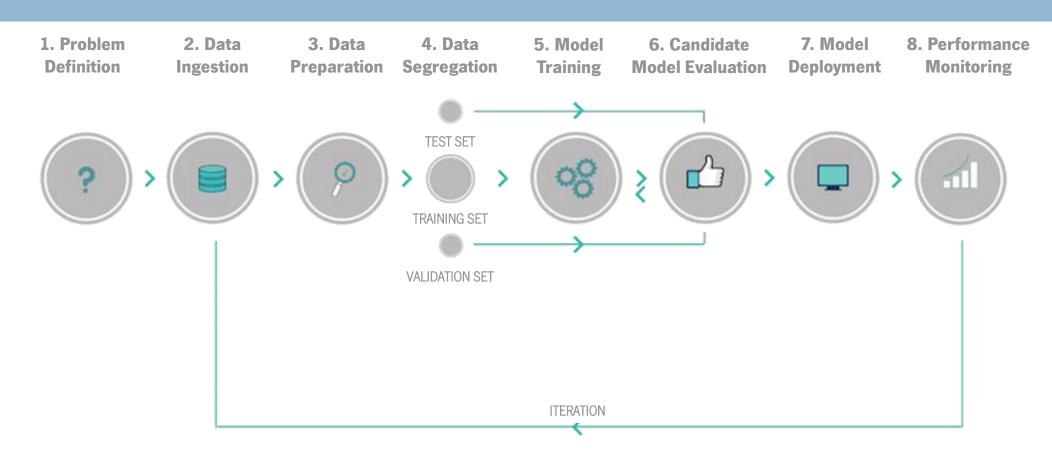
Dados e Aprendizagem Automática

Data Exploration and Preparation

- Understanding The Problem
- Data Exploration
- Data Preparation
- Hands On

Understanding The Problem

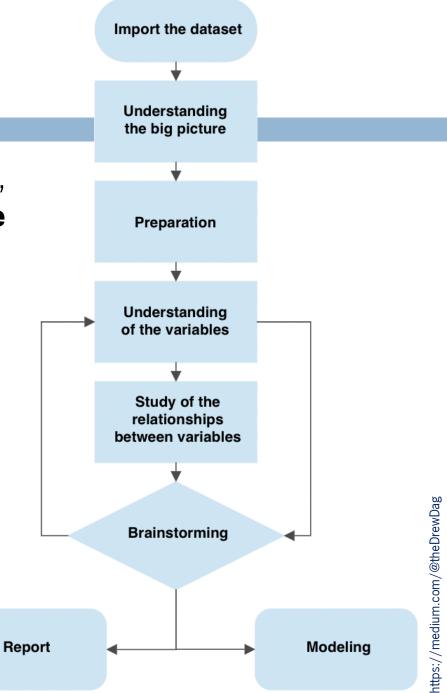
Understanding The Problem



We need to look at our data and understand it.

Understanding the data is a huge step in the process and, as such, will take time. Nevertheless, it will give us a flavour of our dataset, each variable, its meaning and its relevance to this problem.

Let's understand the type of features, how important it can be, if it is described in another feature, etc. Let's use the **wine dataset** available here: https://tinyurl.com/4cshpfac



Imports

Let's import the necessary libraries:

```
import sklearn as skl
import numpy as np
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:

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

df.head()

Data Exploration

What about actual data? What can we **see/learn/understand** from this data?

	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

C

ui.t	all()													
	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 3 5	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, which refer to the type of wine.

There are **no null values**, and the attributes are all numeric except for the Class.

df.dtypes Alcohol float64 Malic acid float64 float64 Ash Alcalinity of ash float64 int64 Magnesium float64 Total phenols Flavanoids float64 Nonflavanoid phenols float64 Proanthocyanins float64 Color intensity float64 float64 Hue OD280/OD315 of diluted wines float64 Proline int64 Class object dtype: object

```
df.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 178 entries, 0 to 177
Data columns (total 14 columns):
                                   Non-Null Count Dtype
     Column
     Alcohol
                                   178 non-null
                                                   float64
     Malic acid
                                   178 non-null
                                                   float64
                                                   float64
     Ash
                                   178 non-null
     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
                                   178 non-null
                                                   float64
     Proanthocyanins
                                                   float64
                                   178 non-null
     Color intensity
                                                   float64
                                   178 non-null
     Hue
                                   178 non-null
                                                   float64
     OD280/OD315 of diluted wines 178 non-null
                                                   float64
     Proline
                                                   int64
 12
                                   178 non-null
    Class
                                   178 non-null
                                                   object
 13
dtypes: float64(11), int64(2), object(1)
memory usage: 19.6+ KB
```

We can also get some descriptive statistics (for all numeric data or only desired):

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?

<pre>df.isna().any()</pre>	
Alcohol	False
Malic acid	False
Ash	False
Alcalinity of ash	False
Magnesium	False
Total phenols	False
Flavanoids	False
Nonflavanoid phenols	False
Proanthocyanins	False
Color intensity	False
Hue	False
OD280/OD315 of diluted wines	False
Proline	False
Class	False
dtype: bool	

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

Our analysis allows us to better characterize the dataset:

- It has 178 entries
- **14 attributes** 13 are physicochemical properties of the wine and 1 is the classification
- All non-null values
- There are no missing values

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

It consists of several steps. Often (in fact, a lot of times), you will need to check the API of the library you are using.

Here are some links you can save for future reference:

- Numpy (https://numpy.org/doc/stable/)
- Pandas (https://pandas.pydata.org/docs/)
- Matplotlib (https://matplotlib.org/stable/users/index.html)
- **Seaborn** (https://seaborn.pydata.org/api.html)
- Scikit Learn (https://scikit-learn.org/stable/api/index.html)

And here are some basic Pandas functions that you will need (sometime) in the future for data preparation:

```
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
```

```
Some basic Sklearn functions/classes you will need as well:
    sklearn.preprocessing.MinMaxScaler
    sklearn.preprocessing.StandardScaler
    sklearn.preprocessing.KBinsDiscretizer
    sklearn.preprocessing.LabelEncoder
    sklearn.feature_selection
    sklearn.metrics
```

Data Preparation and Transformation

Remove duplicate values

```
print(df.duplicated().sum())
print(df.drop duplicates(inplace=True))
print(df.info())
None
<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
                                                   float64
                                   178 non-null
     Ash
                                   178 non-null
                                                   float64
     Alcalinity of ash
                                   178 non-null
                                                   float64
     Magnesium
                                   178 non-null
                                                    int64
    Total phenols
                                                   float64
                                   178 non-null
     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
 12 Proline
                                   178 non-null
                                                    int64
                                                   object
 13 Class
                                   178 non-null
dtypes: float64(11), int64(2), object(1)
memory usage: 19.6+ KB
None
```

Rename attributes

```
df.rename(columns={"OD280/OD315 of diluted wines": "Protein Concentration"}, inplace=True)
df.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 178 entries, 0 to 177
Data columns (total 14 columns):
                            Non-Null Count Dtype
     Column
     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
                            178 non-null
                                            float64
     Color intensity
                            178 non-null
                                            float64
 10
    Hue
                            178 non-null
                                            float64
 11 Protein Concentration 178 non-null
                                            float64
 12 Proline
                            178 non-null
                                            int64
    Class
                                            object
                            178 non-null
dtypes: float64(11), int64(2), object(1)
memory usage: 19.6+ KB
```

Data Preparation and Transformation

```
df_clean = df.drop(df.loc[(df['Ash']<2) & (df['Alcalinity of ash']>15)].index)
print(df_clean)
```

As all the variables appear to be physicochemical measures, they could all be useful and help to define the segmentation of the wine type. There is **no reason to remove columns**.

1											
1	Alcohol	Malic acid	Ash	Alcal	linity	of ash	Magn	esium	Total phe	nols	\
0	14.23	1.71	2.43			15.6		127		2.80	
1	13.20	1.78	2.14			11.2		100		2.65	
2	13.16	2.36	2.67			18.6		101		2.80	
3	14.37	1.95	2.50			16.8		113		3.85	
4	13.24	2.59	2.87			21.0		118		2.80	
173	13.71	5.65	2.45			20.5		95		1.68	
174	13.40	3.91	2.48			23.0		102		1.80	
175	13.27	4.28	2.26			20.0		120		1.59	
176	13.17	2.59	2.37			20.0		120		1.65	
177	14.13	4.10	2.74			24.5		96		2.05	
	Flavanoi	ds Nonflava	noid p	henols	s Proa	anthocya	anins	Color	intensity	, Hue	\
0	3.6	96		0.28	3	-	2.29		5.64	1.04	
1	2.7	76		0.26	5		1.28		4.38	1.05	
2	3.2	24		0.36	9		2.81		5.68	1.03	
3	3.4	49		0.24	4		2.18		7.80	0.86	;
4	2.6	59		0.39	Э		1.82		4.32	1.04	
173	0.6	51		0.52	2		1.06		7.70	0.64	
174	0.7	75		0.43	3		1.41		7.30	0.70	
175	0.6	59		0.43	3		1.35		10.20	0.59	
176	0.6	58		0.53	3		1.46		9.30	0.60	
177	0.7	76		0.56	5		1.35		9.20	0.61	
	Protein (Concentration	n Pro	line	Class						
0		3.9		1065	one						
1		3.4		1050	one						
2		3.1		1185	one						
3		3.4		1480	one						
4		2.9		735	one						
173		1.7			three						
174		1.5			three						
175		1.5	6	835	three						
176		1.6	2	840	three						
177		1.6	0	560	three						

[164 rows x 14 columns]

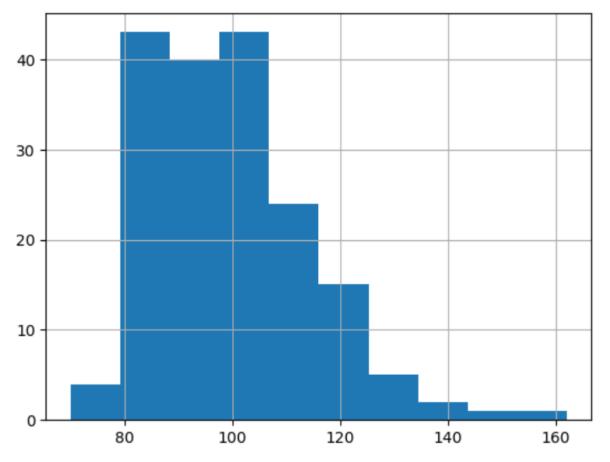
Get basic information by iterating through each relevant variable:

```
df['Alcohol'].value_counts()
Alcohol
13.05
         6
12.37
         6
12.08
12.29
12.42
         3
13.72
         1
13.29
13.74
13.77
         1
14.13
Name: count, Length: 126, dtype: int64
```

```
df['Class'].value counts(normalize=True)
Class
         0.398876
two
         0.331461
one
three
         0.269663
Name: proportion, dtype: float64
111
Numeric variables
111
df['Magnesium'].describe()
         178.000000
count
          99.741573
mean
std
          14.282484
min
          70.000000
25%
          88.000000
50%
          98.000000
75%
         107.000000
         162.000000
max
Name: Magnesium, dtype: float64
```

```
print(f"Histogram: {df['Magnesium'].hist()}")
```

Histogram: Axes(0.125,0.11;0.775x0.77)

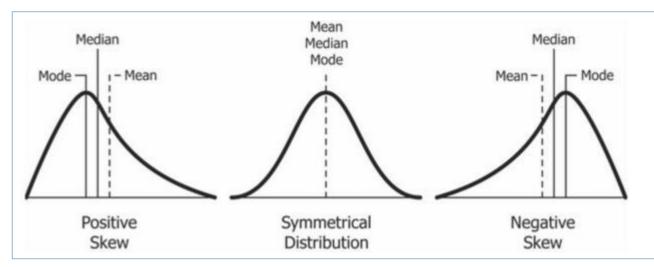


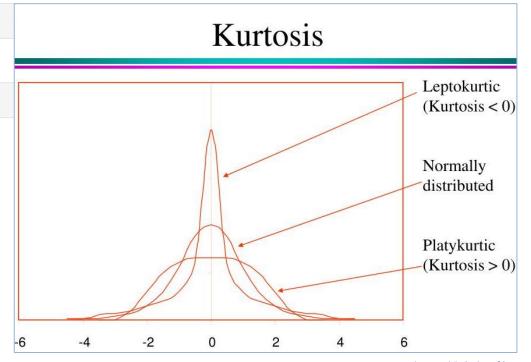
Does **not follow a normal curve** and **has spikes**.

```
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.





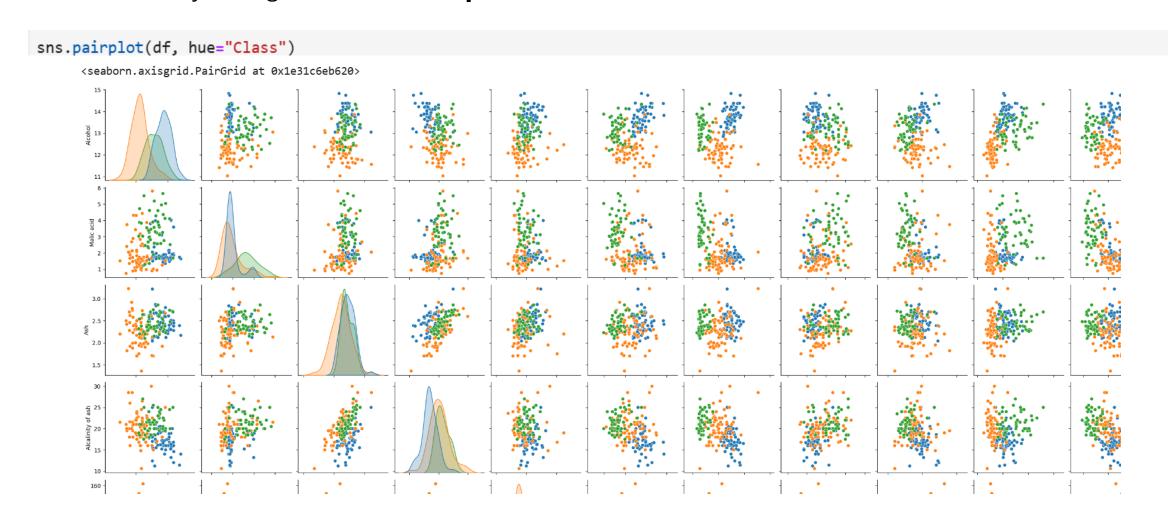
https://t.ly/us-2l

https://t.ly/rlSUJ

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

- **Variable**: the name of the variable
- *Type*: the type or format of the variable. This can be categorical, numerical, Boolean, etc.
- **Context**: useful information to understand the semantic space of the variable. In the case of our dataset, the context is always the physicochemical one
- Expectation: how relevant is this variable for our task? We can use a scale "High, Medium, Low"
- **Comments**: if we have any comments to make about the variable

We can start by looking at the **relationship** between all the variables:



We can **group** by variables:

df.gro	upby(by=['Class']).mo	ean(numer	ric_only=True)									
	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins	Color intensity	Hue	Protein Concentration	Proline
Class													
one	13.744746	2.010678	2.455593	17.037288	106.338983	2.840169	2.982373	0.290000	1.899322	5.528305	1.062034	3.157797	1115.711864
three	13.153750	3.333750	2.437083	21.416667	99.312500	1.678750	0.781458	0.447500	1.153542	7.396250	0.682708	1.683542	629.895833
two	12.278732	1.932676	2.244789	20.238028	94.549296	2.258873	2.080845	0.363662	1.630282	3.086620	1.056282	2.785352	519.507042

df.groupby(by=['Class', 'Proline']).mean(numeric_only=True)

		Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins	Color intensity	Hue	Protein Concentration
Class	Proline												
one	680	13.240	3.980	2.290	17.5	103.0	2.640	2.630	0.32	1.66	4.360	0.820	3.00
	735	13.240	2.590	2.870	21.0	118.0	2.800	2.690	0.39	1.82	4.320	1.040	2.93
	760	14.220	3.990	2.510	13.2	128.0	3.000	3.040	0.20	2.08	5.100	0.890	3.53
	770	12.930	3.800	2.650	18.6	102.0	2.410	2.410	0.25	1.98	4.500	1.030	3.52
	780	14.060	1.630	2.280	16.0	126.0	3.000	3.170	0.24	2.10	5.650	1.090	3.71
two	750	12.835	0.965	2.155	15.9	123.0	2.215	1.575	0.45	1.59	3.285	1.040	2.12
	870	12.290	1.610	2.210	20.4	103.0	1.100	1.020	0.37	1.46	3.050	0.906	1.82
	886	11.960	1.090	2.300	21.0	101.0	3.380	2.140	0.13	1.65	3.210	0.990	3.13
	937	12.470	1.520	2.200	19.0	162.0	2.500	2.270	0.32	3.28	2.600	1.160	2.63
	985	12.990	1.670	2.600	30.0	139.0	3.300	2.890	0.21	1.96	3.350	1.310	3.50

138 rows × 12 columns

print(df	groupby(by=['Alcohol']).agg	g([pd.Serie	s.mode])))		
	Malic acid	Ash	Alcalinity	of ash	Magnesium	Total phenols	\
	mode	mode		mode	mode	mode	
Alcohol							
11.03	1.51	2.2		21.5	85	2.46	
11.41	0.74	2.5		21.0	88	2.48	
11.45	2.4	2.42		20.0	96	2.9	
11.46	3.74	1.82		19.5	107	3.18	
11.56	2.05	3.23		28.5	119	3.18	
14.37	1.95	2.5		16.8	113	3.85	
14.38	[1.87, 3.59]	[2.28, 2.38]	[12.0	, 16.0]	102	[3.25, 3.3]	
14.39	1.87	2.45		14.6	96	2.5	
14.75	1.73	2.39		11.4	91	3.1	
14.83	1.64	2.17		14.0	97	2.8	
	Flavanoids	Nonflavanoid	ohenols Pro	anthocya	nins Color	intensity \	
	mode	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	mode		mode	mode	
Alcohol							
11.03	2.17		0.52		2.01	1.9	
11.41	2.01		0.42		1.44	3.08	
11.45	2.79		0.32		1.83	3.25	
11.46	2.58		0.24		3.58	2.9	
11.56	5.08		0.47		1.87	6.0	
14.37	3.49		0.24		2.18	7.8	
14.38	[3.17, 3.64]	[0.27]	, 0.29]	[2.19, 2	2.96]	[4.9, 7.5]	
14.39	2.52		0.3	_	1.98	5.25	
14.75	3.69		0.43		2.81	5.4	
14.83	2.98		0.29		1.98	5.2	

print(df.groupby(by=['Alcohol', 'Flavanoids']).mean(numeric_only=True)) Malic acid Ash Alcalinity of ash Magnesium \ Alcohol Flavanoids 2.17 1.51 2.20 21.5 85.0 11.03 11.41 0.74 2.50 88.0 2.01 21.0 11.45 2.79 2.40 2.42 20.0 96.0 11.46 2.58 3.74 1.82 107.0 19.5 11.56 5.08 2.05 3.23 28.5 119.0 3.59 2.28 14.38 3.17 16.0 102.0 3.64 1.87 2.38 12.0 102.0 14.39 2.52 1.87 2.45 14.6 96.0 14.75 3.69 1.73 2.39 91.0 11.4 14.83 2.98 1.64 2.17 97.0 14.0 Total phenols Nonflavanoid phenols Proanthocyanins \ Alcohol Flavanoids 11.03 2.17 2.46 0.52 2.01 11.41 2.01 2.48 0.42 1.44 11.45 2.79 2.90 0.32 1.83 11.46 2.58 3.18 0.24 3.58 11.56 5.08 3.18 0.47 1.87 14.38 3.17 3.25 0.27 2.19 3.64 3.30 0.29 2.96 2.52 2.50 0.30 1.98 14.39 14.75 3.10 0.43 2.81 3.69 14.83 2.98 2.80 0.29 1.98

We can create **bins**.

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

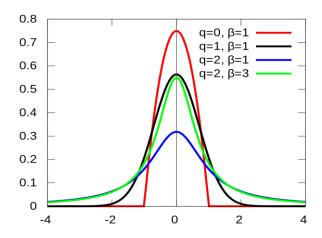
Binning is a **data smoothing technique**. Data smoothing is **used to remove noise from data**.

```
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
0.0
                                                                     59
1.0
                     58
                                 58
                                                         58
                                                                     58
2.0
                                                                     61
                Total phenols Flavanoids Nonflavanoid phenols \
alcohol binned
0.0
                                                              59
1.0
                                       58
                                                              58
2.0
                           61
                                       61
                                                              61
                Proanthocyanins Color intensity Hue Protein Concentration \
alcohol binned
0.0
                             59
                                                                           59
                                                   59
1.0
                             58
                                              58
                                                   58
                                                                           58
2.0
                                              61
                                                                           61
                Proline Class
alcohol binned
0.0
                            59
1.0
                            58
2.0
                            61
```

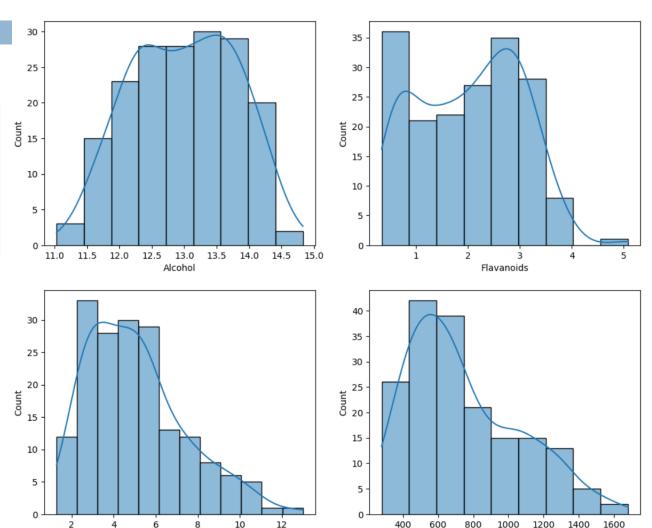
Dispersion: does it follow a Gaussian distribution?

```
fig, axs = plt.subplots(2, 2, figsize=(12, 10))
fig.suptitle('Histograms')

sns.histplot(df['Alcohol'], ax=axs[0, 0], kde=True)
sns.histplot(df['Flavanoids'], ax=axs[0, 1], kde=True)
sns.histplot(df['Color intensity'], ax=axs[1, 0], kde=True)
sns.histplot(df['Proline'], ax=axs[1, 1], kde=True)
```



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



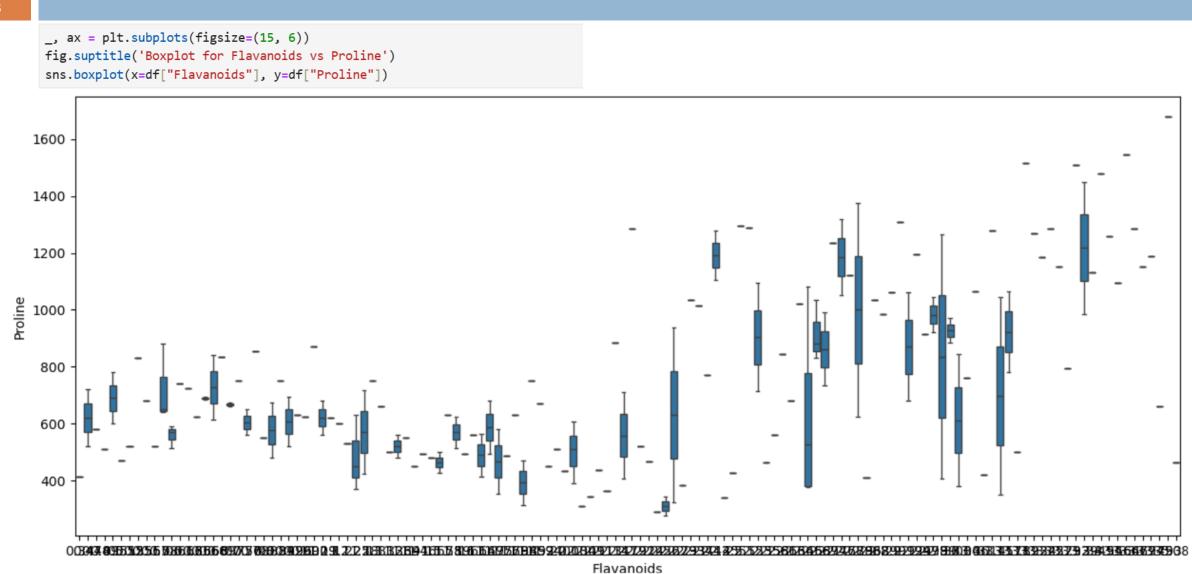
Proline

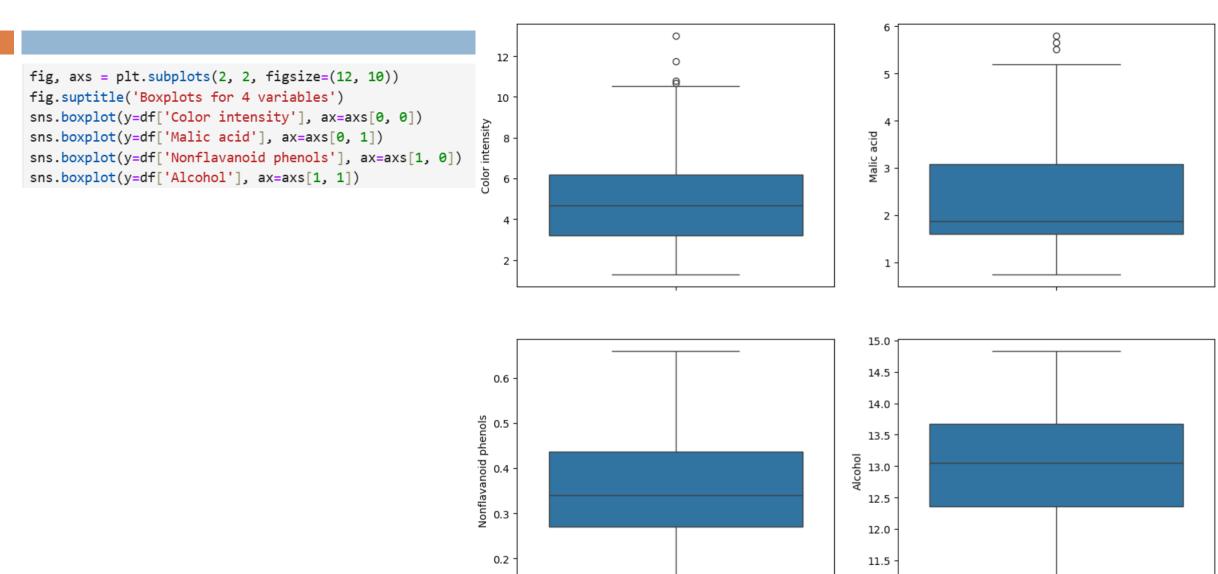
The best way to understand the relationship between a numeric variable and a categorical variable is through a boxplot:

```
plt.title("Boxplot for Class vs Proline")
      plt.show()
                                   Boxplot for Class vs Proline
  1600
  1400
  1200
Poline
1000
   800
    600
   400
                                                                          three
                                               two
                    one
                                               Class
```

sns.catplot(x="Class", y="Proline", data=df, kind="box", aspect=1.5)

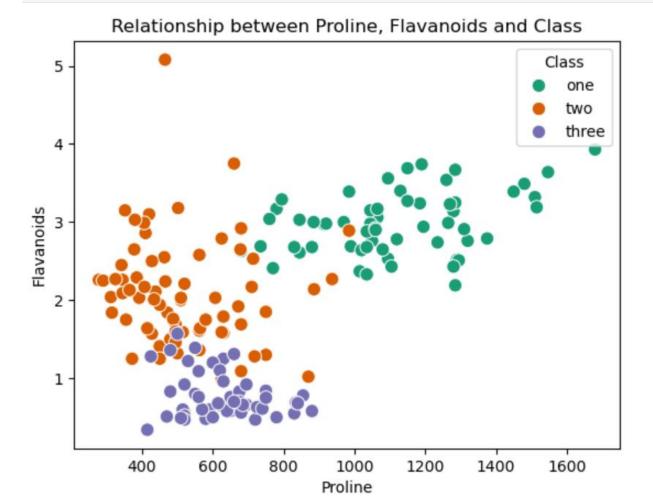
```
sns.catplot(x="Class", y="Flavanoids", data=df, kind="box", aspect=1.5)
    plt.title("Boxplot for Class vs Flavanoids")
    plt.show()
                              Boxplot for Class vs Flavanoids
Flavanoids
w
                                                                        three
                 one
                                             two
                                            Class
```





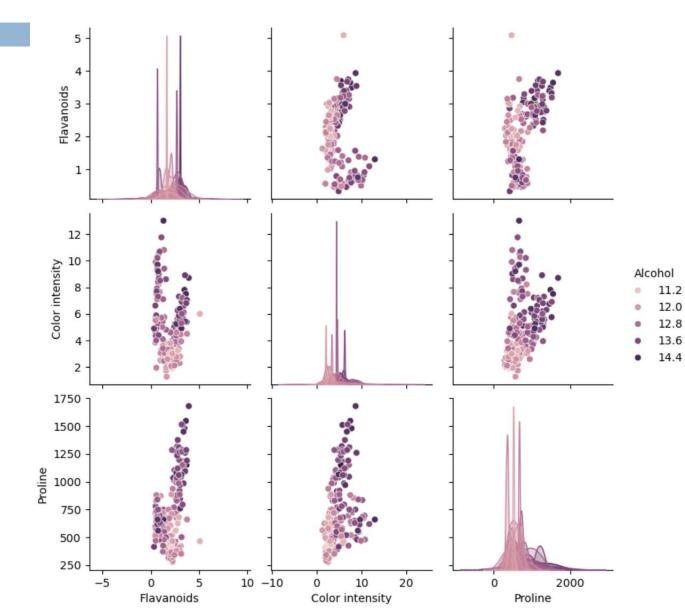
11.0

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



In Class one, Proline levels are much **higher**, while Flavanoids levels are **stable** around the value of 3.

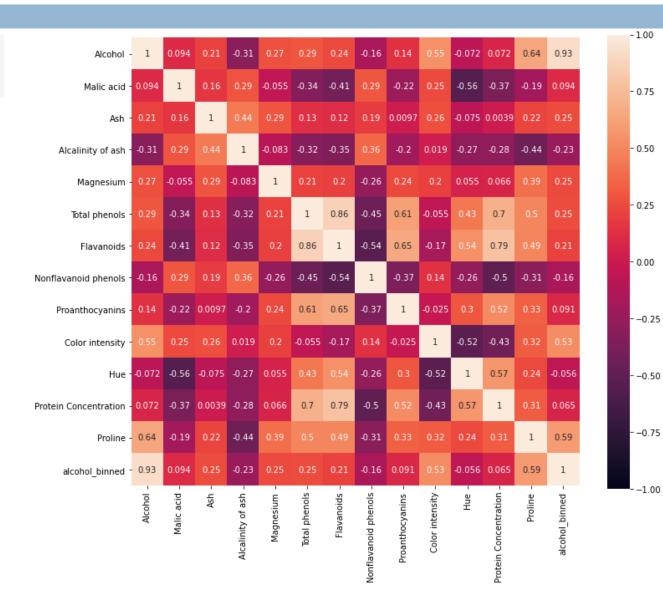
```
cols = ['Alcohol', 'Flavanoids', 'Color intensity', 'Proline']
_ = sns.pairplot(df[cols], hue='Alcohol', height = 2.5)
```



```
corr_matrix = df.corr(numeric_only=True)
f, ax = plt.subplots(figsize=(6,4))
sns.heatmap(corr_matrix, vmin=-1, vmax=1, square=True, annot=True)
```

When the Class variable **decreases** (tends to go to 0), Flavanoids, Total phenols, Proline and other proteins tend to **increase**. And vice versa.

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 different types of wine?
- Which component is the most important?

Hands On