

1. Cleaning and Exploration

In [4]:

```
import pandas as pd
```

In [5]:

```
wine=pd.read_csv(r'C:\Users\DIVYANJALI\Downloads\Wine.csv')
wine.head()
```

Out[5]:

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocya
0	14.23	1.71	2.43	15.6	127	2.80	3.06	0.28	
1	13.20	1.78	2.14	11.2	100	2.65	2.76	0.26	
2	13.16	2.36	2.67	18.6	101	2.80	3.24	0.30	
3	14.37	1.95	2.50	16.8	113	3.85	3.49	0.24	
4	13.24	2.59	2.87	21.0	118	2.80	2.69	0.39	

In [6]:

```
wine.isna().sum()
```

Out[6]:

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
dtype: int64	

In [7]:

```
wine.duplicated()
```

Out[7]:

```
0      False
1      False
2      False
3      False
4      False
...
173     False
174     False
175     False
176     False
177     False
Length: 178, dtype: bool
```

In [9]:

```
wine.describe()
```

Out[9]:

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nitrogen
count	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	1.041905
std	0.811827	1.117146	0.274344	3.339564	14.282484	0.625851	0.998859	0.336174
min	11.030000	0.740000	1.360000	10.600000	70.000000	0.980000	0.340000	0.510000
25%	12.362500	1.602500	2.210000	17.200000	88.000000	1.742500	1.205000	0.700000
50%	13.050000	1.865000	2.360000	19.500000	98.000000	2.355000	2.135000	0.900000
75%	13.677500	3.082500	2.557500	21.500000	107.000000	2.800000	2.875000	1.100000
max	14.830000	5.800000	3.230000	30.000000	162.000000	3.880000	5.080000	1.640000



In [10]:

```
wine.nunique()
```

Out[10]:

Alcohol	126
Malic acid	133
Ash	79
Alcalinity of ash	63
Magnesium	53
Total phenols	97
Flavanoids	132
Nonflavanoid phenols	39
Proanthocyanins	101
Color intensity	132
Hue	78
OD280/OD315 of diluted wines	122
Proline	121

dtype: int64

In [11]:

```
wine.dtypes
```

Out[11]:

Alcohol	float64
Malic acid	float64
Ash	float64
Alcalinity of ash	float64
Magnesium	int64
Total phenols	float64
Flavanoids	float64
Nonflavanoid phenols	float64
Proanthocyanins	float64
Color intensity	float64
Hue	float64
OD280/OD315 of diluted wines	float64
Proline	int64

dtype: object

In [12]:

```
wine.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 178 entries, 0 to 177
Data columns (total 13 columns):
 #   Column                                Non-Null Count  Dtype
---  -
 0   Alcohol                             178 non-null    float64
 1   Malic acid                           178 non-null    float64
 2   Ash                                  178 non-null    float64
 3   Alcalinity of ash                   178 non-null    float64
 4   Magnesium                           178 non-null    int64
 5   Total phenols                       178 non-null    float64
 6   Flavanoids                          178 non-null    float64
 7   Nonflavanoid phenols                178 non-null    float64
 8   Proanthocyanins                    178 non-null    float64
 9   Color intensity                     178 non-null    float64
10   Hue                                 178 non-null    float64
11   OD280/OD315 of diluted wines       178 non-null    float64
12   Proline                             178 non-null    int64
dtypes: float64(11), int64(2)
memory usage: 18.2 KB
```

In [13]:

```
wine.shape
```

Out[13]:

```
(178, 13)
```

In [14]:

```
len(wine)
```

Out[14]:

```
178
```

In [15]:

```
wine.columns
```

Out[15]:

```
Index(['Alcohol', 'Malic acid', 'Ash', 'Alcalinity of ash', 'Magnesium',
      'Total phenols', 'Flavanoids', 'Nonflavanoid phenols',
      'Proanthocyanins', 'Color intensity', 'Hue',
      'OD280/OD315 of diluted wines', 'Proline'],
      dtype='object')
```

In [16]:

```
len(wine.columns)
```

Out[16]:

13

In [17]:

```
wine.size
```

Out[17]:

2314

In [18]:

```
wine.tail()
```

Out[18]:

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins
173	13.71	5.65	2.45	20.5	95	1.68	0.61	0.52	
174	13.40	3.91	2.48	23.0	102	1.80	0.75	0.43	
175	13.27	4.28	2.26	20.0	120	1.59	0.69	0.43	
176	13.17	2.59	2.37	20.0	120	1.65	0.68	0.53	
177	14.13	4.10	2.74	24.5	96	2.05	0.76	0.56	



In [19]:

```
wine.corr()
```

Out[19]:

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids
Alcohol	1.000000	0.094397	0.211545	-0.310235	0.270798	0.289101	0.236815
Malic acid	0.094397	1.000000	0.164045	0.288500	-0.054575	-0.335167	-0.411007
Ash	0.211545	0.164045	1.000000	0.443367	0.286587	0.128980	0.115077
Alcalinity of ash	-0.310235	0.288500	0.443367	1.000000	-0.083333	-0.321113	-0.351370
Magnesium	0.270798	-0.054575	0.286587	-0.083333	1.000000	0.214401	0.195784
Total phenols	0.289101	-0.335167	0.128980	-0.321113	0.214401	1.000000	0.864564
Flavanoids	0.236815	-0.411007	0.115077	-0.351370	0.195784	0.864564	1.000000
Nonflavanoid phenols	-0.155929	0.292977	0.186230	0.361922	-0.256294	-0.449935	-0.537900
Proanthocyanins	0.136698	-0.220746	0.009652	-0.197327	0.236441	0.612413	0.652692
Color intensity	0.546364	0.248985	0.258887	0.018732	0.199950	-0.055136	-0.172379
Hue	-0.071747	-0.561296	-0.074667	-0.273955	0.055398	0.433681	0.543479
OD280/OD315 of diluted wines	0.072343	-0.368710	0.003911	-0.276769	0.066004	0.699949	0.787194
Proline	0.643720	-0.192011	0.223626	-0.440597	0.393351	0.498115	0.494193

2. Univariate EDA

In [20]:

```
import matplotlib.pyplot as plt
import seaborn as sns
import numpy as np
%matplotlib inline

import warnings
warnings.filterwarnings("ignore")
```

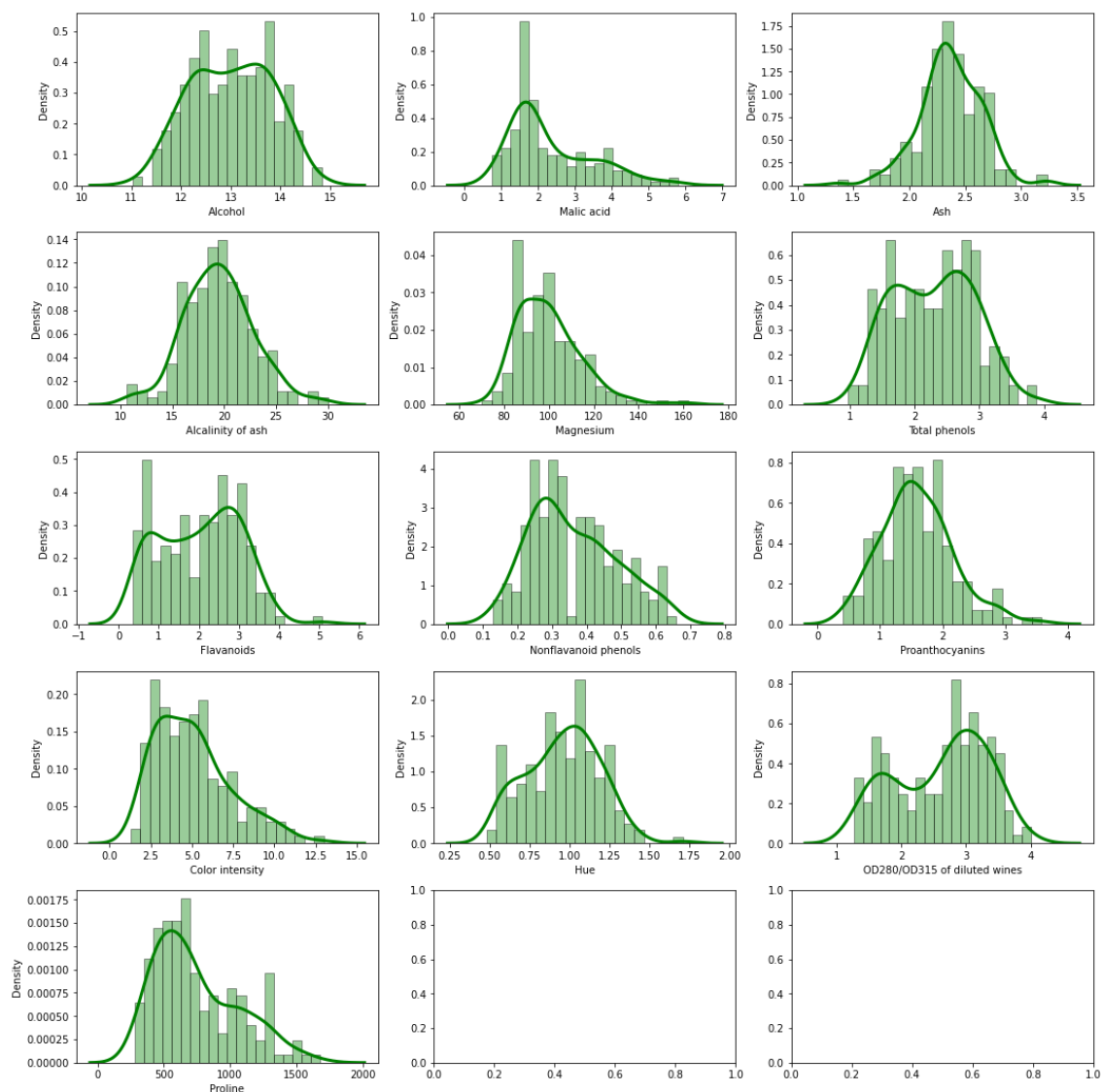
In [21]:

```
rows=5
cols=3
fig,ax=plt.subplots(nrows=rows,ncols=cols,figsize=(15,15))
col=wine.columns
index=0
for i in range(rows):
    for j in range(cols):
        sns.distplot(wine[col[index]], ax=ax[i][j],
                      color='green', bins=20,
                      hist_kws={'edgecolor':'black'},
                      kde_kws={'linewidth':3})
        index=index+1
    if index>=12:
        break
plt.tight_layout()
```

```
'''Here we can conclude that, Alkalinity of ash, Magnesium and Proanthocyanins approximately follows Normal distribution.\nAlcohol, Malic acid, Total Phenols, Flavanoids, Hue, OD280/OD315 and Proline of diluted wines\nsuggests the presence of 2 clusters.'''
```

Out[21]:

```
'Here we can conclude that, Alkalinity of ash, Magnesium and Proanthocyanins approximately follows Normal distribution.\nAlcohol, Malic acid, Total Phenols, Flavanoids, Hue, OD280/OD315 and Proline of diluted wines\nsuggests the presence of 2 clusters.'
```



In []:

```
# Alcohol, OD280/OD315 of diluted wines and Ash are negatively skewed. The other variables a
```

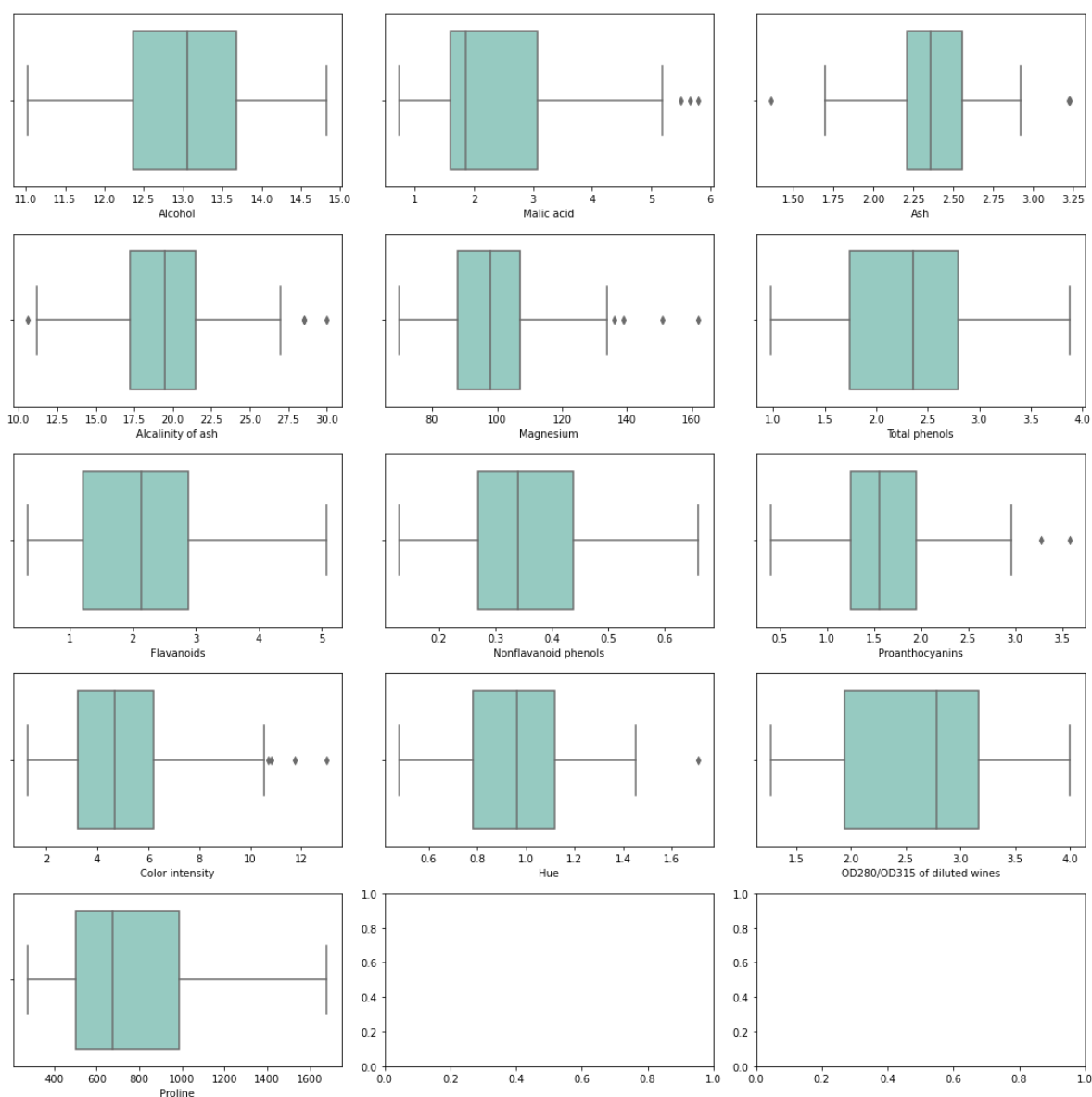

In [22]:

```
rows=5
cols=3
fig,ax=plt.subplots(nrows=rows,ncols=cols,figsize=(15,15))
col=wine.columns
index=0
for i in range(rows):
    for j in range(cols):
        sns.boxplot(wine[col[index]],ax=ax[i][j], palette="Set3")
        index=index+1
        if index>=12:
            break
plt.tight_layout()

'''From the boxplots we observe that the variables
Malic acid, Ash, Alcalinity of Ash, Magnesium, Proanthocyanins, Color intensity, Hue
seem to have outliers'''
```

Out[22]:

'From the boxplots we observe that the variables \nMalic acid, Ash, Alcalini
ty of Ash, Magnesium, Proanthocyanins, Color intensity, Hue \nseem to have o
utliers'



In []:

```
# From the boxplots we observe the variables Malic acid, Ash, Alcalinity of Ash, Magnesium,  
# Color intensity, Hue seem to have outliers.
```

3. Multivariate EDA

In []:

```
rows=2  
cols=6  
fig,ax=plt.subplots(nrows=rows,ncols=cols,figsize=(15,5))  
col=wine.columns  
index=0  
for i in range(rows):  
    for j in range(cols):  
        sns.kdeplot(x=wine["Alcohol"],y=wine[col[index+1]],ax=ax[i][j],  
                    shade=True, color='red')  
        index=index+1  
plt.tight_layout()
```

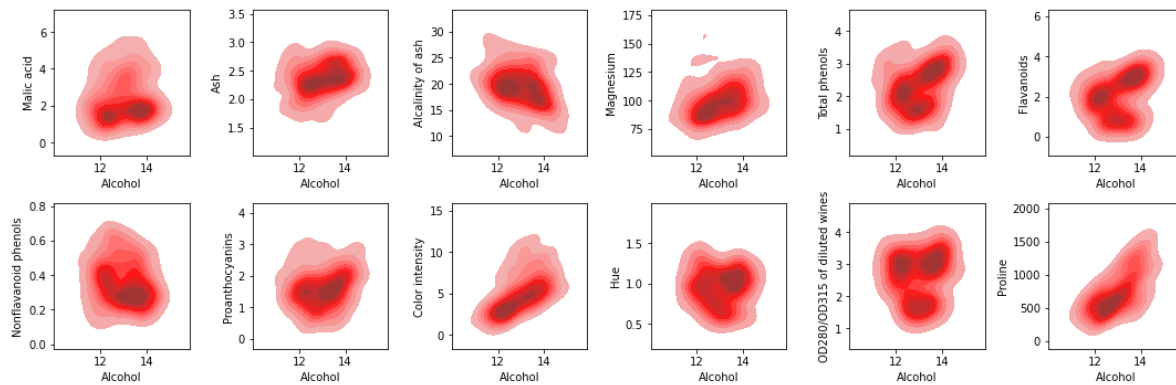
In [23]:

```
#Alcohol
rows=2
cols=6
fig,ax=plt.subplots(nrows=rows,ncols=cols,figsize=(15,5))
col=wine.columns
index=0
for i in range(rows):
    for j in range(cols):
        sns.kdeplot(x=wine["Alcohol"],y=wine[col[index+1]],ax=ax[i][j],
                    shade=True, color='red')
        index=index+1
plt.tight_layout()

'''From the bivariate Kdeplots it can be said that there might be 2 or 3 clusters.'''
```

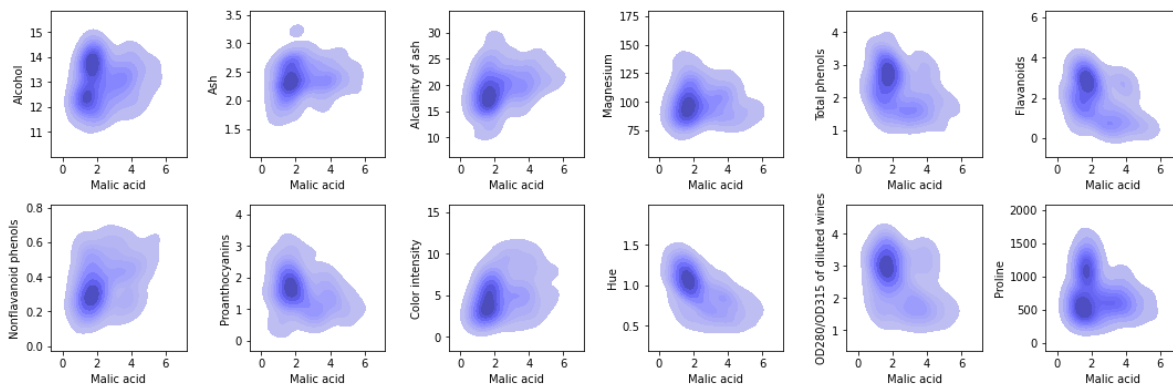
Out[23]:

'From the bivariate Kdeplots it can be said that there might be 2 or 3 clusters.'



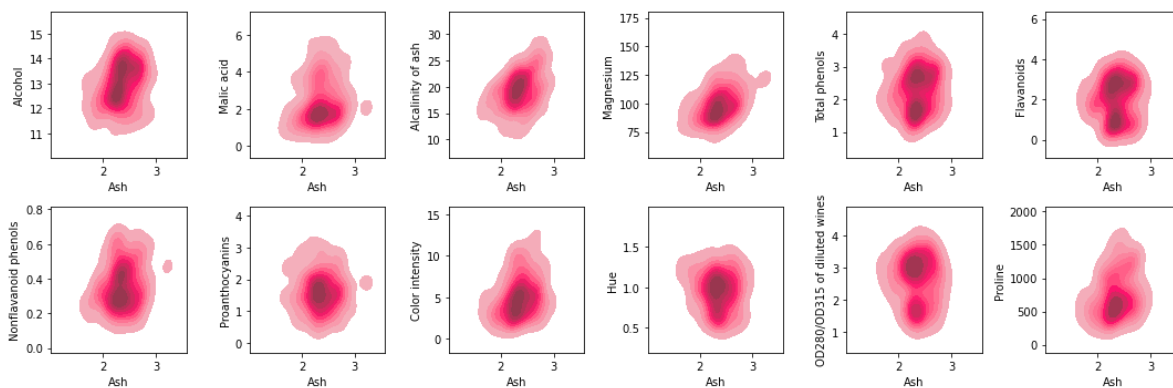
In [24]:

```
#Malic Acid
rows=2
cols=6
fig,ax=plt.subplots(nrows=rows,ncols=cols,figsize=(15,5))
col=wine.columns
index=0
for i in range(rows):
    for j in range(cols):
        if index==0:
            sns.kdeplot(x=wine["Malic acid"],y=wine[col[index]],ax=ax[i][j],
                        shade=True, color='blue')
        else:
            sns.kdeplot(x=wine["Malic acid"],y=wine[col[index+1]],ax=ax[i][j],
                        shade=True, color='blue')
        index=index+1
plt.tight_layout()
```



In [25]:

```
#Ash
rows=2
cols=6
fig,ax=plt.subplots(nrows=rows,ncols=cols,figsize=(15,5))
col=wine.columns
index=0
for i in range(rows):
    for j in range(cols):
        if index in range(0,2):
            sns.kdeplot(x=wine["Ash"],y=wine[col[index]],ax=ax[i][j],
                        shade=True, color='pink')
        else:
            sns.kdeplot(x=wine["Ash"],y=wine[col[index+1]],ax=ax[i][j],
                        shade=True, color='pink')
        index=index+1
plt.tight_layout()
```

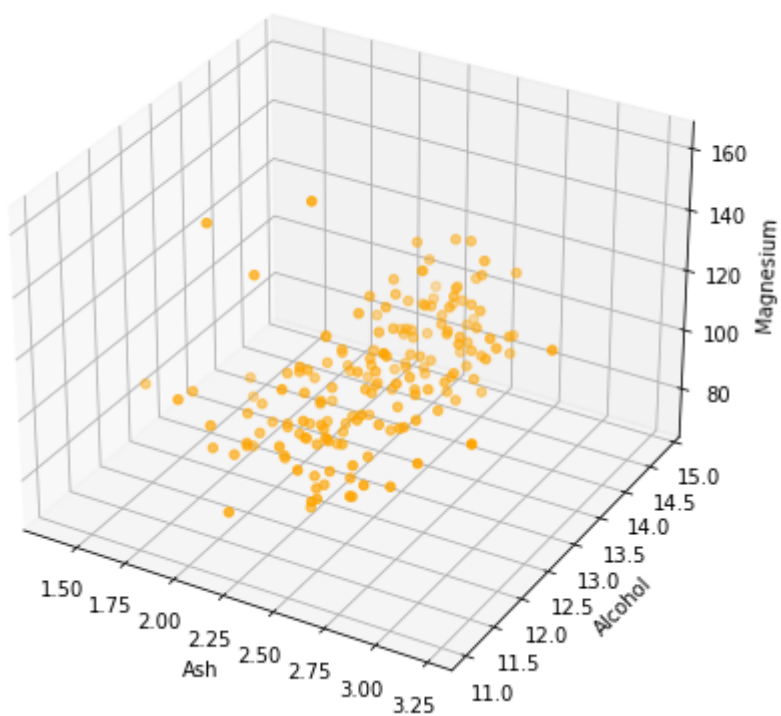


In []:

```
# From the bivariate KDEplots it can be said that there might be two or at maximum 3 cluste
```

In [26]:

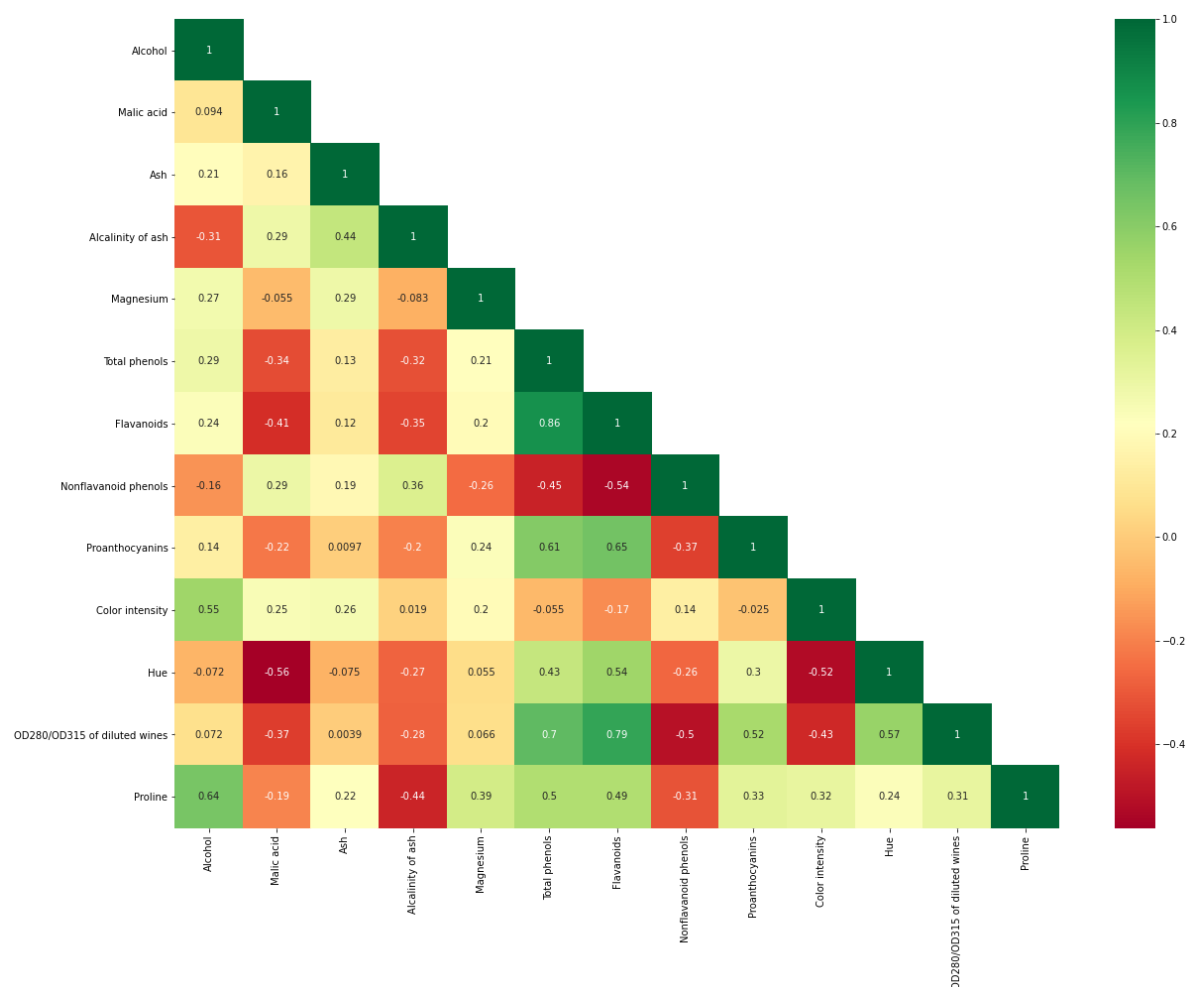
```
fig=plt.figure(figsize=(10,7))
ax=plt.axes(projection='3d')
ax.scatter(wine['Ash'],wine['Alcohol'],wine['Magnesium'], c='orange');
ax.set_xlabel('Ash')
ax.set_ylabel('Alcohol')
ax.set_zlabel("Magnesium");
```



In [27]:

```
plt.figure(figsize=(20,15))
mask = np.triu(np.ones_like(wine.corr(), dtype=bool), k=1)
sns.heatmap(wine.corr(), annot=True, cmap='RdYlGn', mask=mask);
```

*#there seems to be a high correlation between Flavanoids and total phenols
#and Flavanoids and OD280/OD315 of diluted wines.*



In [28]:

```
for a in range(len(wine.corr().columns)):
    for b in range(a):
        if abs(wine.corr().iloc[a,b]>0.7):
            name=wine.corr().columns[a]
            print(name)
```

Flavanoids

OD280/OD315 of diluted wines

- Removing outliers

In [29]:

```
def outliers(df, ft):
    Q1=df[ft].quantile(0.25)
    Q3=df[ft].quantile(0.75)
    IQR=Q3-Q1
    lower_bound=Q1-(IQR*1.5)
    upper_bound=Q3+(IQR*1.5)
    ls=df.index[ (df[ft]<lower_bound) | (df[ft]>upper_bound) ]
    return ls
```

In [30]:

```
index_list=[]
for feature in wine.keys():
    index_list.extend(outliers(wine, feature))
print(index_list, end='')
```

[123, 137, 173, 25, 59, 121, 59, 73, 121, 127, 69, 73, 78, 95, 95, 110, 151,
158, 159, 166, 115]

In [31]:

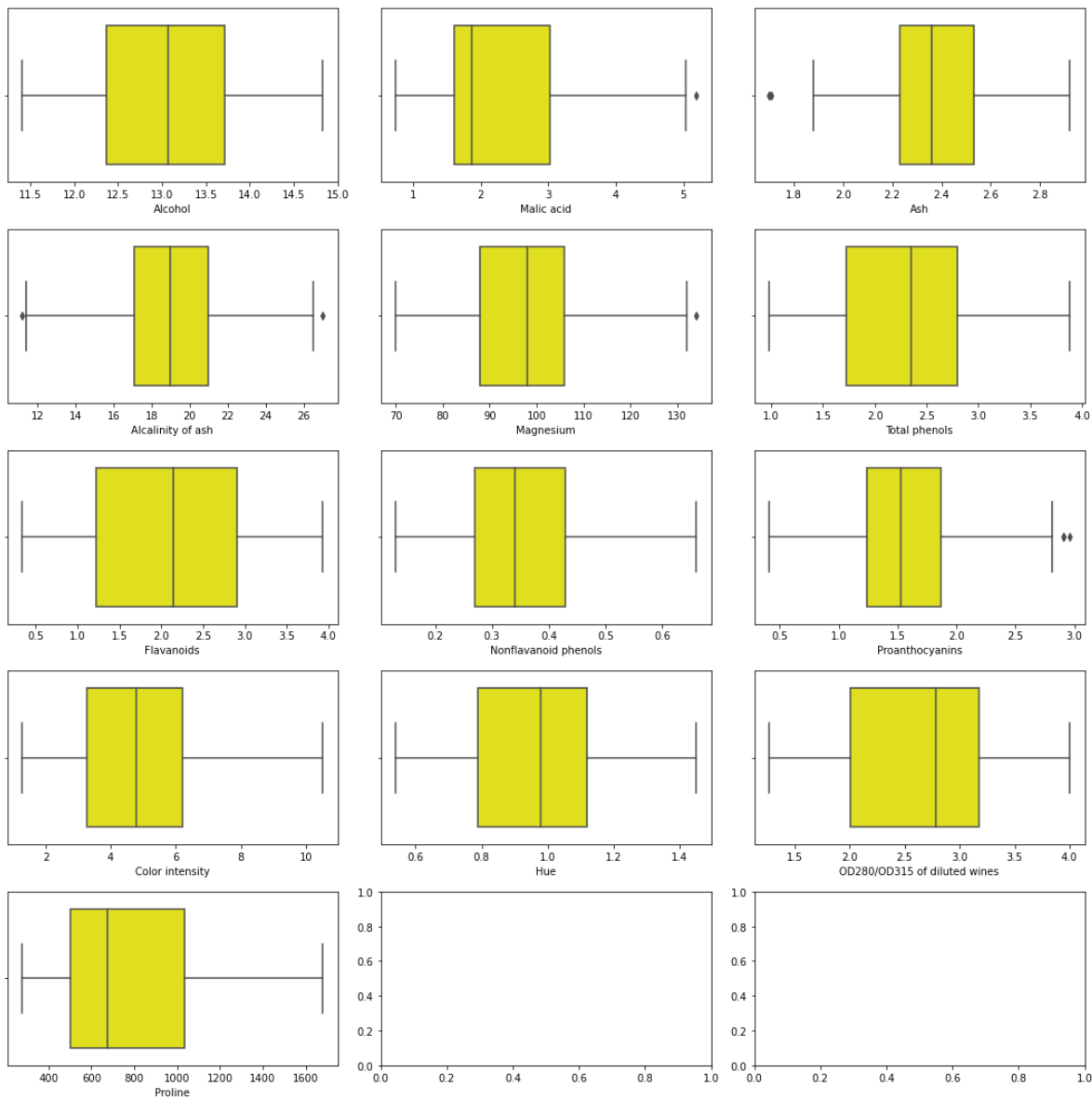
```
def remove(df, ls):
    ls=sorted(set(ls))
    df=df.drop(ls)
    return df
wine_cleaned=remove(wine, index_list)
wine_cleaned.shape
```

Out[31]:

(161, 13)

In [32]:

```
rows=5
cols=3
fig,ax=plt.subplots(nrows=rows,ncols=cols,figsize=(15,15))
col=wine_cleaned.columns
index=0
for i in range(rows):
    for j in range(cols):
        sns.boxplot(wine_cleaned[col[index]],ax=ax[i][j], color='yellow')
        index=index+1
    if index>=12:
        break
plt.tight_layout()
```

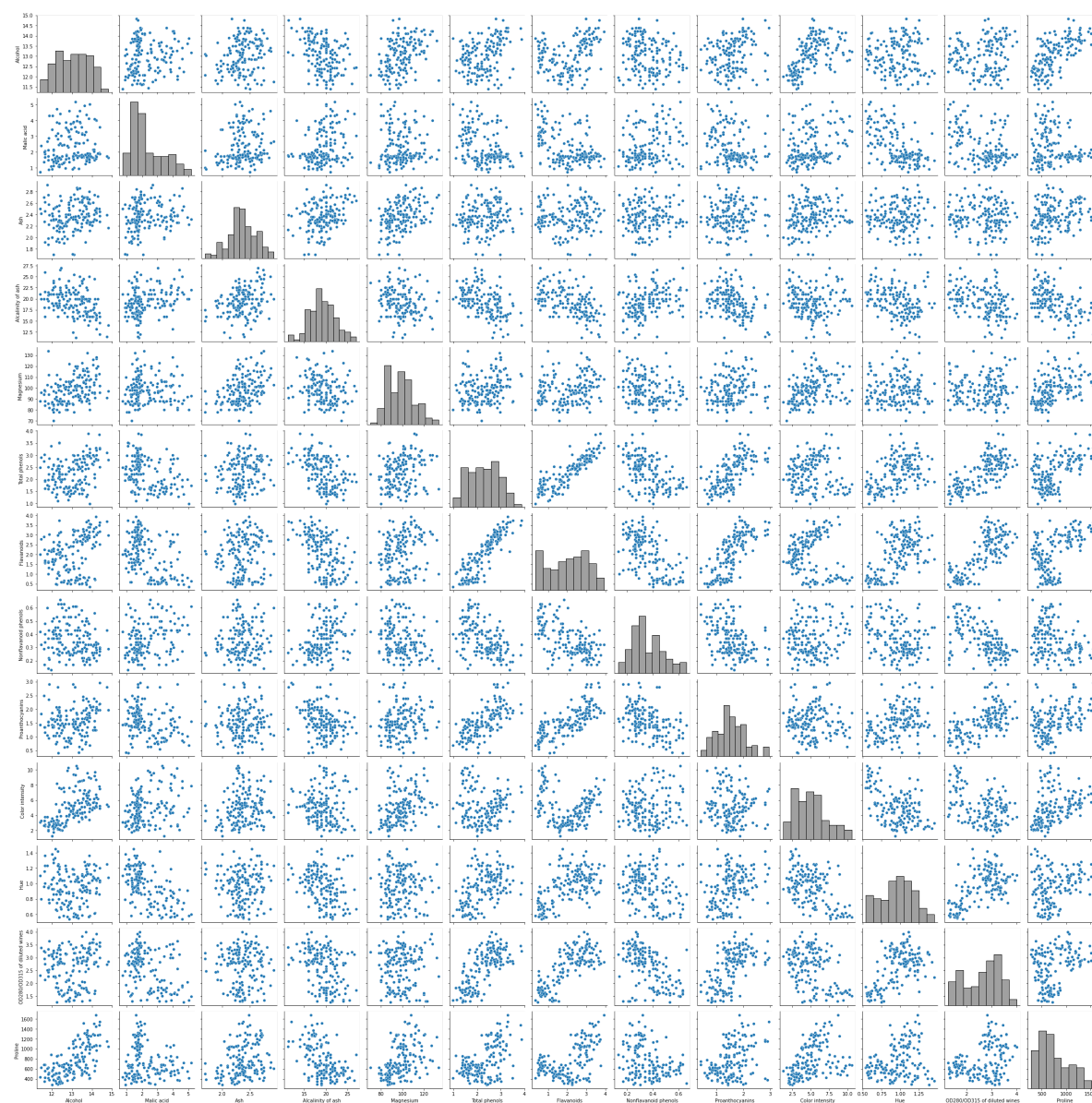


In [33]:

```
sns.pairplot(wine_cleaned, diag_kws={'color':'grey'})
```

Out[33]:

<seaborn.axisgrid.PairGrid at 0x1db533469a0>



Principal Component Analysis

In [34]:

```
x=wine_cleaned

#standardisation
from sklearn.preprocessing import StandardScaler
sc= StandardScaler()
x_scaled=pd.DataFrame(sc.fit_transform(x), columns=x.columns)
x_scaled.head(2)
```

Out[34]:

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols
0	1.495711	-0.571130	0.277425	-1.208619	2.309259	0.808420	1.034224	-0.643463
1	0.200698	-0.504145	-0.928625	-2.672685	0.118914	0.570475	0.728906	-0.808165

In [35]:

```
#PCA
from sklearn.decomposition import PCA
pca=PCA()
x_pca1=pd.DataFrame(pca.fit_transform(x_scaled), columns=x_scaled.columns)
x_pca1.head(2)
```

Out[35]:

	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	Total phenols	Flavanoids	Nonflavanoid phenols
0	3.482298	-1.494604	0.133281	-0.171033	0.650584	-0.512913	-0.733783	0.342958
1	2.278164	0.375183	-1.873077	-0.672753	0.530476	-1.217015	-0.049324	-0.893003

In [36]:

```
pca.explained_variance_ratio_
```

*#The first 5 Principal Components are capturing around 80% of the variance so we can replace with the new 5 features having 80% of the information.
#So, we have reduced the 11 dimensions to only 5 dimensions while retaining most of the information.*

Out[36]:

```
array([0.38853448, 0.20487624, 0.09547051, 0.06919384, 0.05789018,
       0.04289108, 0.03510666, 0.0259047 , 0.02394086, 0.01980589,
       0.0175546 , 0.01308515, 0.00574581])
```

In [37]:

```
#Dimensionality Reduction
pca=PCA(n_components=5)
x_pca2=pd.DataFrame(pca.fit_transform(x_scaled), columns=['PC1', 'PC2', 'PC3', 'PC4', 'PC5'])
x_pca2.head(2)
```

Out[37]:

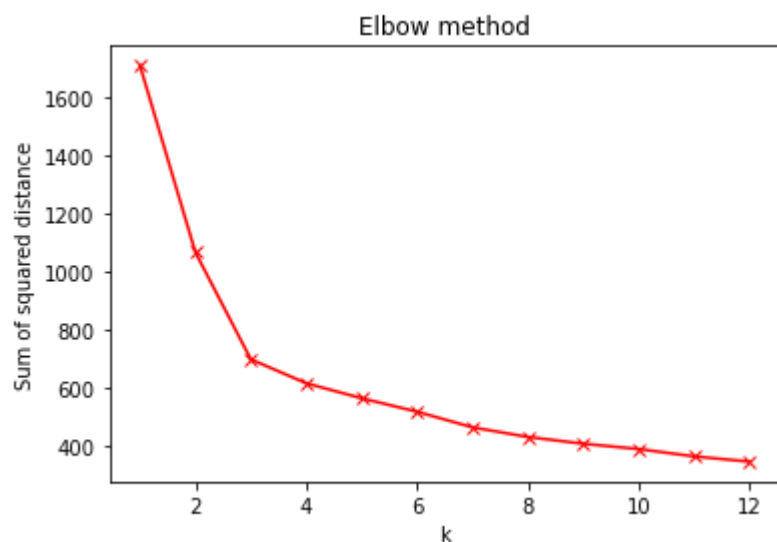
	PC1	PC2	PC3	PC4	PC5
0	3.482298	-1.494604	0.133281	-0.171033	0.650584
1	2.278164	0.375183	-1.873077	-0.672753	0.530476

1. K means clustering

In [38]:

```
from sklearn.cluster import KMeans
ssd=[]
K=range(1,13)
for k in K:
    km=KMeans(n_clusters=k)
    km=km.fit(x_pca2)
    ssd.append(km.inertia_)

plt.plot(K, ssd, 'rx-');
plt.xlabel('k');
plt.ylabel('Sum of squared distance');
plt.title('Elbow method');
```



In []:

```
# Thus, we choose no. of clusters to be 3.
```

In [40]:

```
km=KMeans(n_clusters=3,init='k-means++', random_state=0)
km.fit(x_pca2)
```

Out[40]:

```
KMeans(n_clusters=3, random_state=0)
```

In [41]:

```
centroids=km.cluster_centers_
centroids
```

Out[41]:

```
array([[ 2.38884698, -0.88560974, -0.02554146, -0.08793572, -0.0877621 ],
       [-2.78775617, -1.2489108 , -0.29375436,  0.08181669,  0.03935514],
       [-0.22593271,  1.85459226,  0.25345433,  0.02445725,  0.05722795]])
```

In [42]:

```
km.inertia_
```

Out[42]:

```
699.8420783063123
```

In [43]:

```
labels=km.labels_
labels
```

Out[43]:

```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 1, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1])
```

In [44]:

```
from collections import Counter
Counter(labels)
```

Out[44]:

```
Counter({0: 58, 2: 58, 1: 45})
```

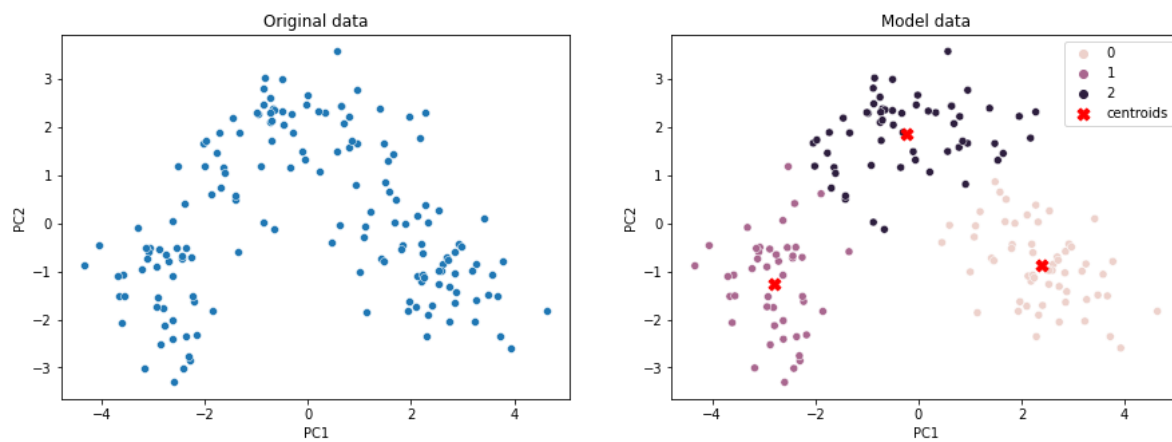
In [45]:

```
#Visualising the clusters using scatter plot
```

```
plt.figure(figsize=(15,5))
ax1=plt.subplot(1,2,1)
ax1.set_title('Original data')
sns.scatterplot(data = x_pca2, x='PC1', y='PC2', ax=ax1);
ax2=plt.subplot(1,2,2)
ax2.set_title('Model data')
sns.scatterplot(data = x_pca2, x='PC1', y='PC2', hue=km.labels_, ax=ax2);
plt.scatter(centroids[:, 0], centroids[:, 1], marker="X", c="r", s=80, label="centroids");
plt.legend()
```

Out[45]:

<matplotlib.legend.Legend at 0x1db5e0c4250>



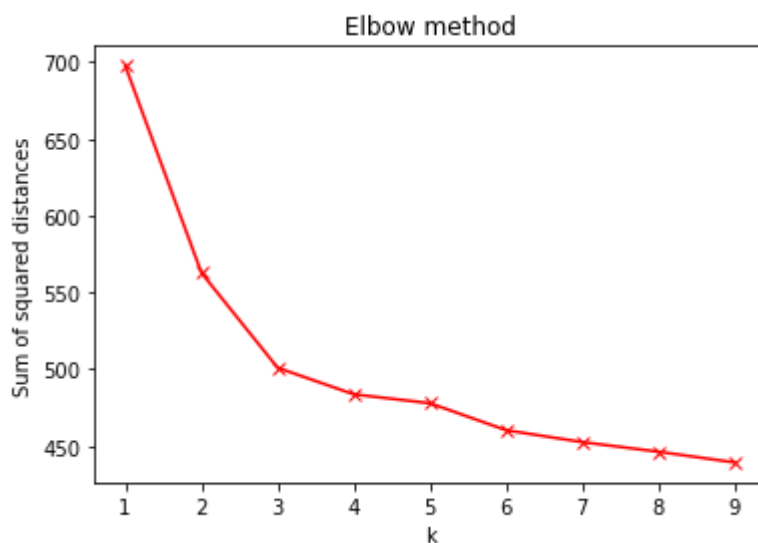
In [47]:

```
from sklearn_extra.cluster import KMedoids
ssd=[]
for k in range(1,10):
    kmed=KMedoids(n_clusters=k, max_iter=300, random_state=1)
    kmed.fit(scaled_wine)
    ssd.append(kmed.inertia_)

plt.plot(range(1,10), ssd, 'rx-');
plt.xlabel('k')
plt.ylabel("Sum of squared distances");
plt.title("Elbow method")
```

Out[47]:

Text(0.5, 1.0, 'Elbow method')



2. K Medoids

In [48]:

```
from sklearn.decomposition import PCA
pca=PCA(n_components=2)
pc=pd.DataFrame(pca.fit_transform(scaled_wine), columns=['PC1', 'PC2'])
pc.head()
```

Out[48]:

	PC1	PC2
0	3.316751	-1.443463
1	2.209465	0.333393
2	2.516740	-1.031151
3	3.757066	-2.756372
4	1.008908	-0.869831

In [58]:

```
kmed=KMedoids(n_clusters=3, random_state=0)
kmed.fit(pc)
'''wine['Labels']=kmed.predict(scaled_wine)
wine.head(2)'''
```

Out[58]:

```
"wine['Labels']=kmed.predict(scaled_wine)\nwine.head(2)"
```

In [59]:

```
centroids=kmed.cluster_centers_
centroids
```

Out[59]:

```
array([[ -0.72328949, -0.23681583],
       [  0.2229686 ,  0.58496601],
       [  0.76943894, -0.38281809]])
```

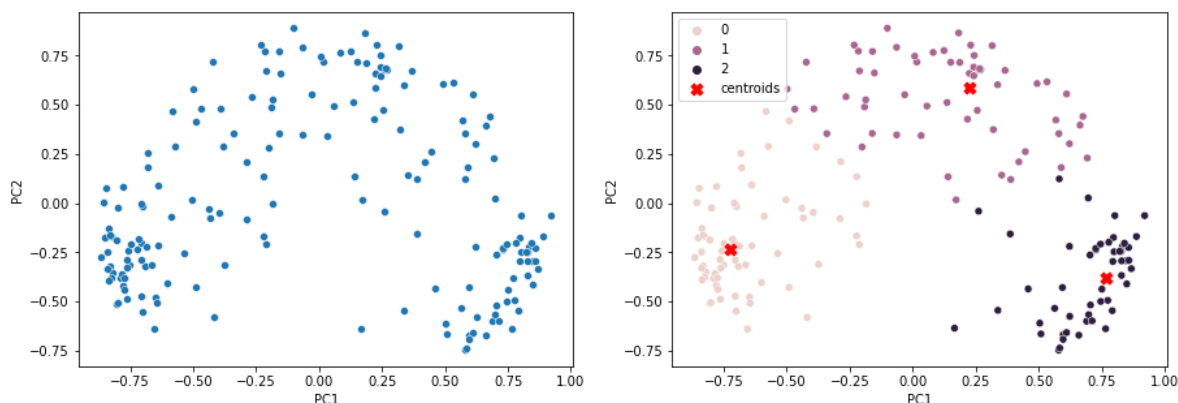
In [60]:

```
plt.figure(figsize=(15,5))
ax1=plt.subplot(1,2,1)
sns.scatterplot(data = pc, x='PC1', y='PC2', ax=ax1);

ax2=plt.subplot(1,2,2)
sns.scatterplot(data = pc, x='PC1', y='PC2',
               ax=ax2, hue=kmed.labels_)
plt.scatter(centroids[:, 0], centroids[:, 1],
           marker="X", c="r", s=80, label="centroids");
plt.legend()
```

Out[60]:

<matplotlib.legend.Legend at 0x1db5f8395e0>



3. Gaussian Mixture clustering

In [61]:

```
from sklearn.preprocessing import StandardScaler, normalize
sc=StandardScaler()
scaled_wine=sc.fit_transform(wine)

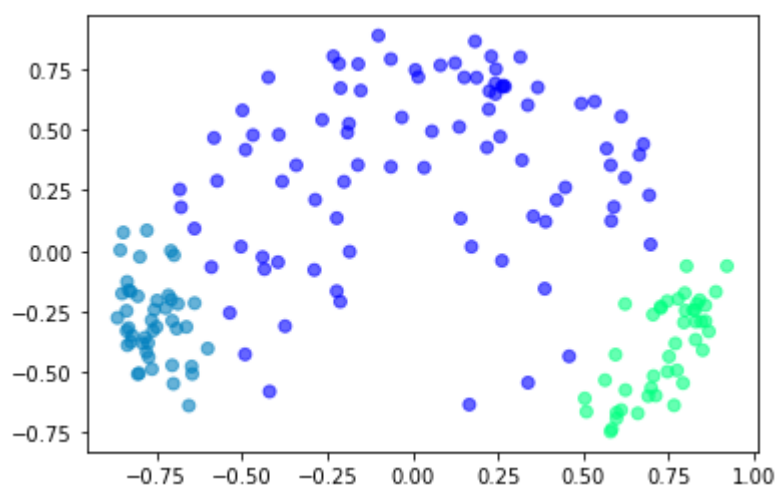
normalised_wine=pd.DataFrame(normalize(scaled_wine))

pca=PCA(n_components=2)
pc=pd.DataFrame(pca.fit_transform(normalised_wine), columns=['PC1', 'PC2'])
print(pc.head(2))

from sklearn.mixture import GaussianMixture
gmm=GaussianMixture(n_components=3)
gmm.fit(pc)
labels=GaussianMixture(n_components=3).fit_predict(pc)

plt.scatter(pc['PC1'], pc['PC2'],
            c = labels, cmap =plt.cm.winter, alpha = 0.6)
plt.show()
```

	PC1	PC2
0	-0.832433	-0.318834
1	-0.639443	0.091947



4. Hierarchical Clustering — Agglomerative Clustering :

In [62]:

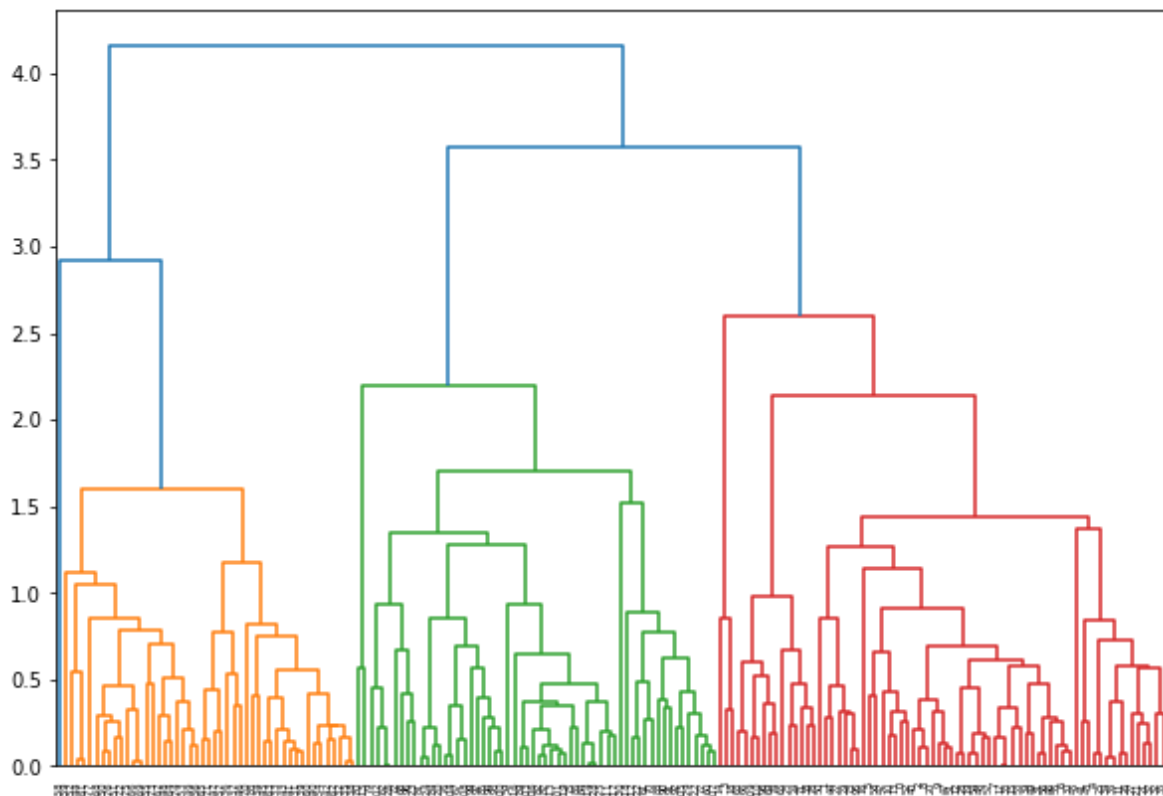
```
from sklearn.preprocessing import StandardScaler, normalize
sc=StandardScaler()
scaled_wine=sc.fit_transform(wine)

pca=PCA(n_components=2)
pc=pd.DataFrame(pca.fit_transform(scaled_wine), columns=['PC1', 'PC2'])
print(pc.head(2))

from scipy.cluster.hierarchy import dendrogram, linkage
plt.figure(figsize=(30,25))
link=linkage(pc, method='centroid')
plt.figure(figsize=(10, 7))
dendrogram(link);
```

	PC1	PC2
0	3.316751	-1.443463
1	2.209465	0.333393

<Figure size 2160x1800 with 0 Axes>

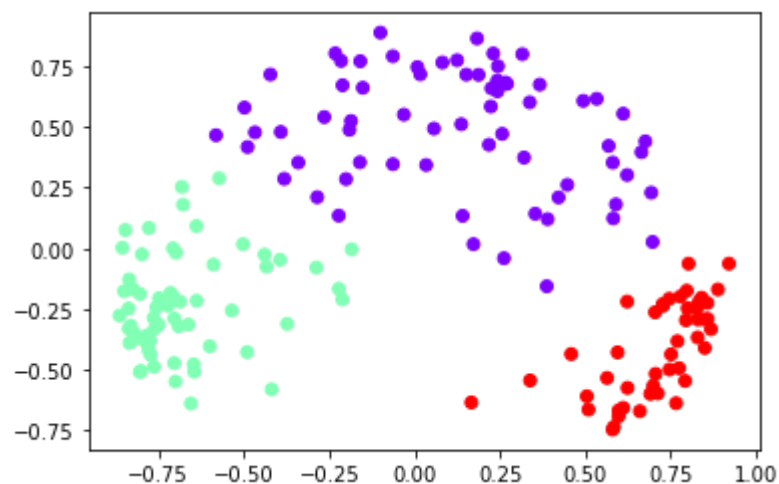


In [69]:

```
from sklearn.cluster import AgglomerativeClustering
agg=AgglomerativeClustering(n_clusters=3, affinity='euclidean', linkage='ward')
agg.fit_predict(pc)
plt.scatter(pc['PC1'], pc['PC2'], c=agg.labels_, cmap='rainbow')
```

Out[69]:

<matplotlib.collections.PathCollection at 0x1db5ff68ca0>



5. Spectral Clustering

In [70]:

```
from sklearn.preprocessing import StandardScaler, normalize
sc=StandardScaler()
scaled_wine=sc.fit_transform(wine)

normalised_wine=normalize(scaled_wine)

from sklearn.decomposition import PCA
pca=PCA(n_components=2)
pc=pd.DataFrame(pca.fit_transform(normalised_wine), columns=['PC1', 'PC2'])

from sklearn.cluster import SpectralClustering
sp=SpectralClustering(n_clusters=3, affinity='rbf')

labels = sp.fit_predict(normalised_wine)

plt.scatter(pc['PC1'],pc['PC2'], c=labels)
```

Out[70]:

<matplotlib.collections.PathCollection at 0x1db5ffd40a0>

