DSC 540- Topic 7- Assignment

September 22, 2021

[80]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.cluster import KMeans
from yellowbrick.cluster import KElbowVisualizer
import seaborn as sns
```

For this assignment I will be using the Wine dataset UCI Machine Learning Repository. The link for the dataset is given below. https://archive.ics.uci.edu/ml/datasets/wine

[205]:
```
# Let's load the Wine dataset in a dataframe and assign the Column names

wine = pd.read_csv('H:/Krishna/GCU/DSC 540/Topic 7/wine.data', sep=',',
 ↪header=None,names=['Type','Alcohol','Malic_Acid','Ash','Ash_Alcanity','Magnesium',
 ↪'Total_Phenols','Flavanoids','Nonflavanoid_Phenols','Proanthocyanins',
 ↪'Color_Intensity','Hue','OD280','Proline'])
wine.describe()
```

[205]:

	Type	Alcohol	Malic_Acid	Ash	Ash_Alcanity	\
count	178.000000	178.000000	178.000000	178.000000	178.000000	
mean	1.938202	13.000618	2.336348	2.366517	19.494944	
std	0.775035	0.811827	1.117146	0.274344	3.339564	
min	1.000000	11.030000	0.740000	1.360000	10.600000	
25%	1.000000	12.362500	1.602500	2.210000	17.200000	
50%	2.000000	13.050000	1.865000	2.360000	19.500000	
75%	3.000000	13.677500	3.082500	2.557500	21.500000	
max	3.000000	14.830000	5.800000	3.230000	30.000000	

	Magnesium	Total_Phenols	Flavanoids	Nonflavanoid_Phenols	\
count	178.000000	178.000000	178.000000	178.000000	
mean	99.741573	2.295112	2.029270	0.361854	
std	14.282484	0.625851	0.998859	0.124453	
min	70.000000	0.980000	0.340000	0.130000	
25%	88.000000	1.742500	1.205000	0.270000	
50%	98.000000	2.355000	2.135000	0.340000	

```
75%     107.000000        2.800000     2.875000              0.437500
max     162.000000        3.880000     5.080000              0.660000

        Proanthocyanins  Color_Intensity         Hue        OD280      Proline
count        178.000000       178.000000  178.000000  178.000000   178.000000
mean           1.590899         5.058090    0.957449    2.611685   746.893258
std            0.572359         2.318286    0.228572    0.709990   314.907474
min            0.410000         1.280000    0.480000    1.270000   278.000000
25%            1.250000         3.220000    0.782500    1.937500   500.500000
50%            1.555000         4.690000    0.965000    2.780000   673.500000
75%            1.950000         6.200000    1.120000    3.170000   985.000000
max            3.580000        13.000000    1.710000    4.000000  1680.000000
```

[192]:
```
wine.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 178 entries, 0 to 177
Data columns (total 14 columns):
 #   Column                Non-Null Count  Dtype
---  ------                --------------  -----
 0   Type                  178 non-null    int64
 1   Alcohol               178 non-null    float64
 2   Malic_Acid            178 non-null    float64
 3   Ash                   178 non-null    float64
 4   Ash_Alcanity          178 non-null    float64
 5   Magnesium             178 non-null    int64
 6   Total_Phenols         178 non-null    float64
 7   Flavanoids            178 non-null    float64
 8   Nonflavanoid_Phenols  178 non-null    float64
 9   Proanthocyanins       178 non-null    float64
 10  Color_Intensity       178 non-null    float64
 11  Hue                   178 non-null    float64
 12  OD280                 178 non-null    float64
 13  Proline               178 non-null    int64
dtypes: float64(11), int64(3)
memory usage: 19.6 KB
```

Before we building the clustering the algorithm, we need to standardise the dataset. From above we can see that the 13 dimensional attributes are all of different values and for a proper model it is advised to standardise the data.

Standardize Dataset

[220]:
```
from sklearn.preprocessing import StandardScaler

# The Stnadardscaler function will help in scaling the data
wine_std = pd.DataFrame(StandardScaler().fit_transform(wine.iloc[:,1:14]))
wine_std.
 ↪columns=['Alcohol','Malic_Acid','Ash','Ash_Alcanity','Magnesium','Total_Phenols',
```

```
␣
↪'Flavanoids','Nonflavanoid_Phenols','Proanthocyanins','Color_Intensity','Hue','OD280','Prol
```

[221]:
```
wine_std.describe()
```

[221]:

	Alcohol	Malic_Acid	Ash	Ash_Alcanity	Magnesium
count	1.780000e+02	1.780000e+02	1.780000e+02	1.780000e+02	1.780000e+02
mean	-8.619821e-16	-8.357859e-17	-8.657245e-16	-1.160121e-16	-1.995907e-17
std	1.002821e+00	1.002821e+00	1.002821e+00	1.002821e+00	1.002821e+00
min	-2.434235e+00	-1.432983e+00	-3.679162e+00	-2.671018e+00	-2.088255e+00
25%	-7.882448e-01	-6.587486e-01	-5.721225e-01	-6.891372e-01	-8.244151e-01
50%	6.099988e-02	-4.231120e-01	-2.382132e-02	1.518295e-03	-1.222817e-01
75%	8.361286e-01	6.697929e-01	6.981085e-01	6.020883e-01	5.096384e-01
max	2.259772e+00	3.109192e+00	3.156325e+00	3.154511e+00	4.371372e+00

	Total_Phenols	Flavanoids	Nonflavanoid_Phenols	Proanthocyanins
count	1.780000e+02	1.780000e+02	1.780000e+02	1.780000e+02
mean	-2.972030e-16	-4.016762e-16	4.079134e-16	-1.699639e-16
std	1.002821e+00	1.002821e+00	1.002821e+00	1.002821e+00
min	-2.107246e+00	-1.695971e+00	-1.868234e+00	-2.069034e+00
25%	-8.854682e-01	-8.275393e-01	-7.401412e-01	-5.972835e-01
50%	9.595986e-02	1.061497e-01	-1.760948e-01	-6.289785e-02
75%	8.089974e-01	8.490851e-01	6.095413e-01	6.291754e-01
max	2.539515e+00	3.062832e+00	2.402403e+00	3.485073e+00

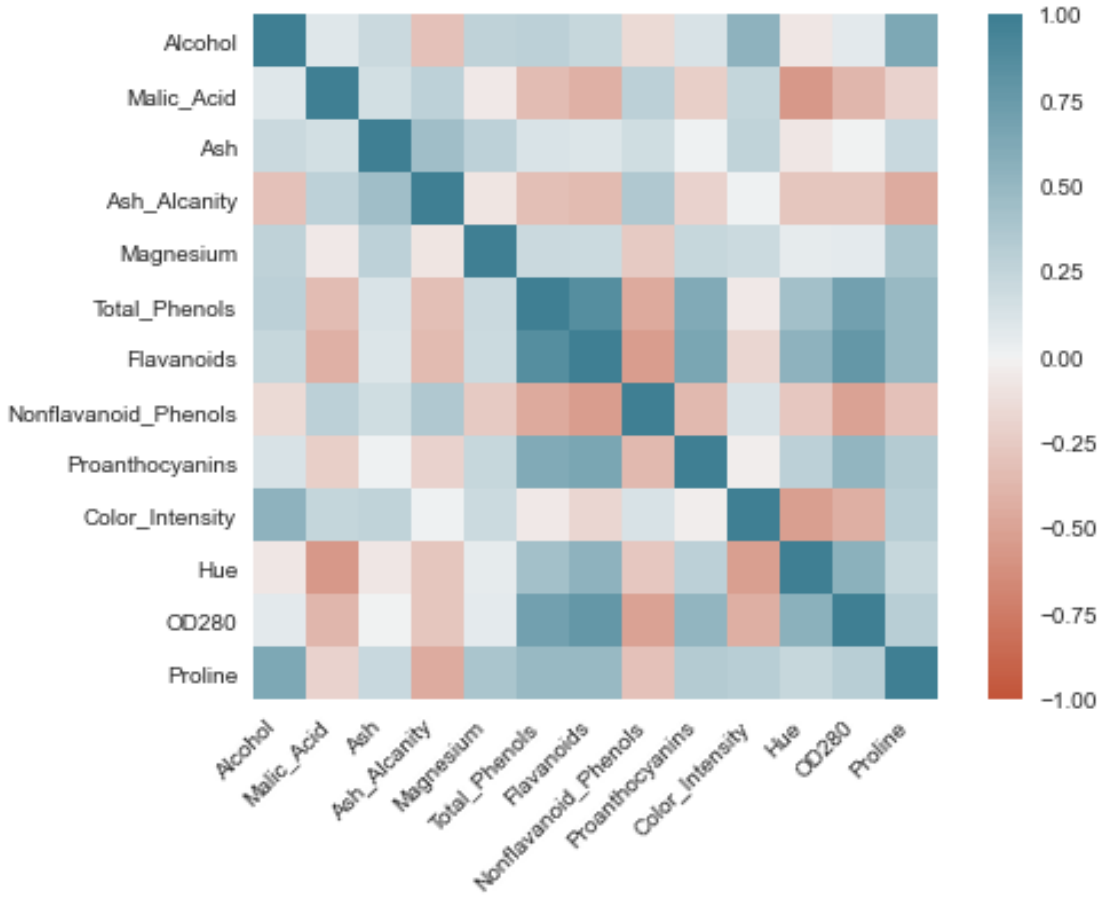
	Color_Intensity	Hue	OD280	Proline
count	1.780000e+02	1.780000e+02	1.780000e+02	1.780000e+02
mean	-1.122697e-17	3.717376e-16	2.919013e-16	-7.484650e-18
std	1.002821e+00	1.002821e+00	1.002821e+00	1.002821e+00
min	-1.634288e+00	-2.094732e+00	-1.895054e+00	-1.493188e+00
25%	-7.951025e-01	-7.675624e-01	-9.522483e-01	-7.846378e-01
50%	-1.592246e-01	3.312687e-02	2.377348e-01	-2.337204e-01
75%	4.939560e-01	7.131644e-01	7.885875e-01	7.582494e-01
max	3.435432e+00	3.301694e+00	1.960915e+00	2.971473e+00

[223]:
```
# Let us split the input data into the Predictor and Response variable
# We have a total of 13 Input variables here. We can try and build a model with␣
↪all the 13 and see how our clusters look
X = wine_std
y = wine.iloc[:,-14]
```

[267]:
```
# Let us use a Correlation matrix to identify how the dimensional variables are␣
↪correlated with each other in our wine dataset
corr=wine_std.iloc[:,0:13].corr()
ax = sns.heatmap(
    corr,
    vmin=-1, vmax=1, center=0,
```

```
    cmap=sns.diverging_palette(20, 220, n=200),
    square=True
)
ax.set_xticklabels(
    ax.get_xticklabels(),
    rotation=45,
    horizontalalignment='right'
)
```

[267]:
```
[Text(0.5, 0, 'Alcohol'),
 Text(1.5, 0, 'Malic_Acid'),
 Text(2.5, 0, 'Ash'),
 Text(3.5, 0, 'Ash_Alcanity'),
 Text(4.5, 0, 'Magnesium'),
 Text(5.5, 0, 'Total_Phenols'),
 Text(6.5, 0, 'Flavanoids'),
 Text(7.5, 0, 'Nonflavanoid_Phenols'),
 Text(8.5, 0, 'Proanthocyanins'),
 Text(9.5, 0, 'Color_Intensity'),
 Text(10.5, 0, 'Hue'),
 Text(11.5, 0, 'OD280'),
 Text(12.5, 0, 'Proline')]
```

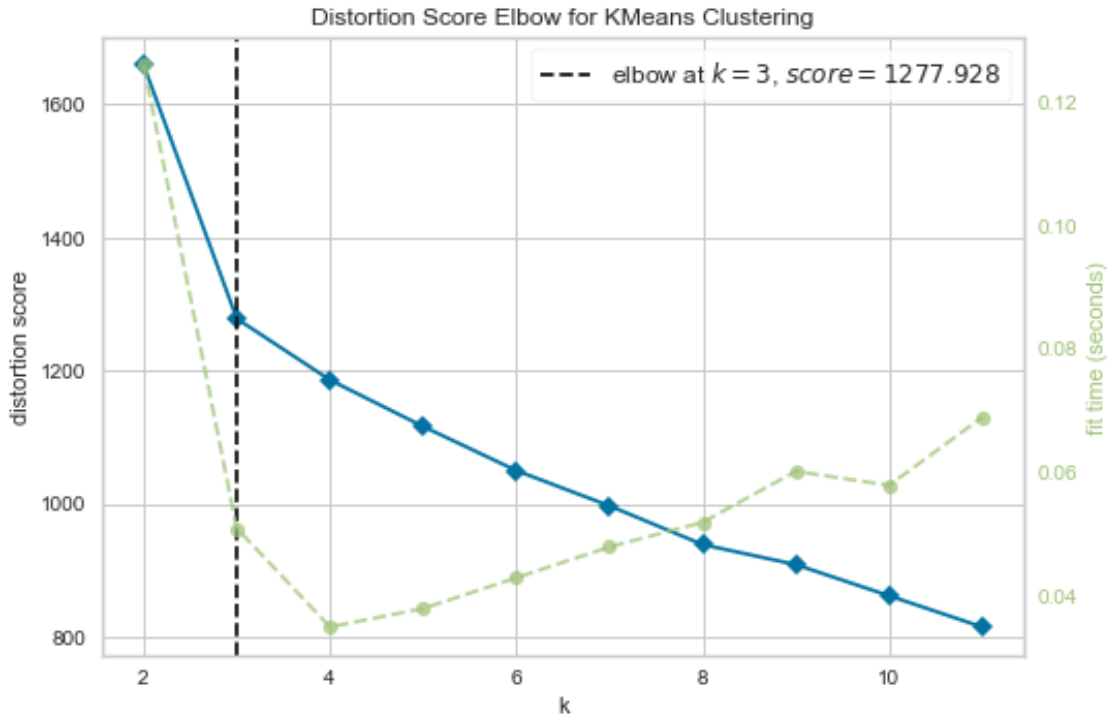


Selecting the Number of Clusters

It is necessary that when we do a k-mean clustering we need to identify the optimal number of clusters. Not selecting the optimal number may often impact the overall efficiency of the model. Below we will use the Kelbow Visaulizer package to find the optimal k that we would need to model our wine data.

[224]:
```
# Let us define the kmean model
model = KMeans()
# In order to identify the cluster we will select between k= 2 to 12 to see␣
 ↪which has the better performance.
# The below function plots the number of k against the sum of squared distance␣
 ↪(distortion) for each k.
visualizer = KElbowVisualizer(model, k=(2,12))
visualizer.fit(X)
visualizer.show()

#Reference: https://www.scikit-yb.org/en/latest/api/cluster/elbow.html
```



[224]:
```
<AxesSubplot:title={'center':'Distortion Score Elbow for KMeans Clustering'},
xlabel='k', ylabel='distortion score'>
```

By looking at the plot above we can very well conclude that the score is highest at k=3. Hence we will use 3 clusters for our k-mean algorithm.

[225]:
```
# Let us build the kmean algorithm using the Kmeans package from the skleran␣
↪package.
# The n_clusters parameter has the number of cluster that need to be classified␣
↪and the max_iter has the maximum number of iterations that is performed in a␣
↪single run
km = KMeans(n_clusters=3,max_iter=300)
y_km = km.fit_predict(X)

wine_std['Pred_Type'] = y_km
```

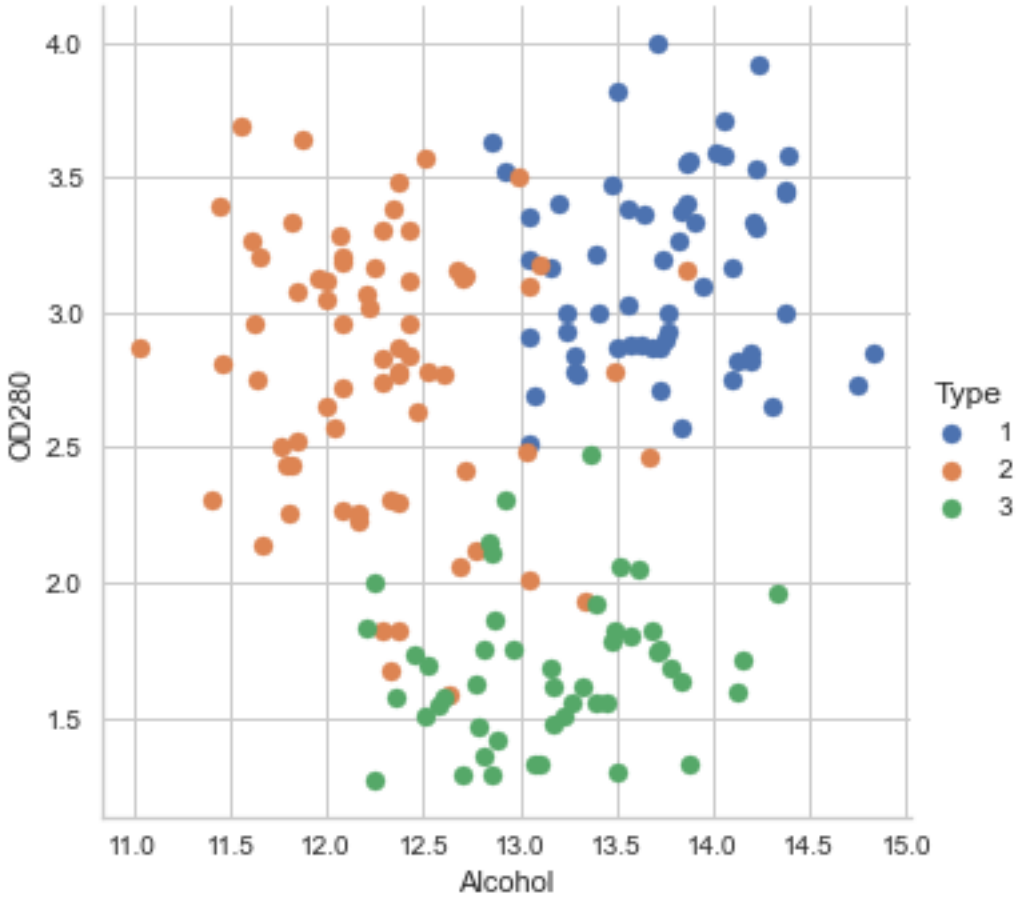
[226]:
```
kmc=km.cluster_centers_
km.n_iter_
```

[226]:
```
10
```

[168]:
```
# Below is the scatter plot of the source data clustered based on the Alcohol␣
↪Type.
```

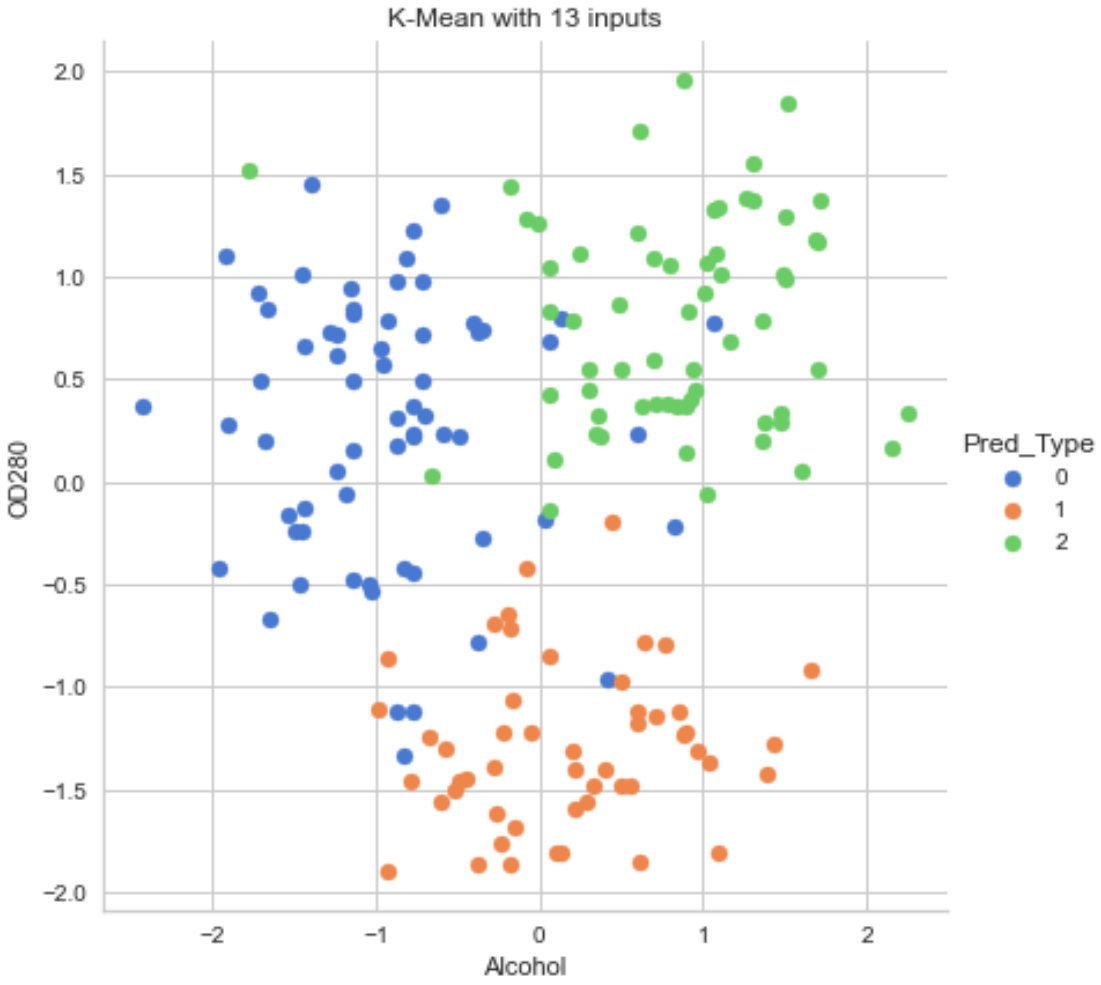
```
sns.FacetGrid(wine, hue="Type", height=5,palette = 'deep').map(plt.
 ↪scatter,'Alcohol','OD280').add_legend()
# We can see 3 clear clusters in the plot.
```

[168]: <seaborn.axisgrid.FacetGrid at 0x13507678d00>



[229]:
```
# Let's plot the outcome of the k-means cluster to see how the data is clustered
sns.FacetGrid(wine_std, hue="Pred_Type", height=6,palette = 'muted').map(plt.
 ↪scatter,'Alcohol','OD280').add_legend()
plt.title('K-Mean with 13 inputs')
# Eventhough we can see three clusters, we do see that there is an overlap of␣
 ↪the clustered groups.
# This is because of the number of input variables selected for our clustering␣
 ↪model.
# In order to get an efficient clustering we need to get the most effective␣
 ↪input variables.
# This can be achieved by the Principal Component Analysis (PCA)
```

[229]: Text(0.5, 1.0, 'K-Mean with 13 inputs')



Principal Component Analysis (PCA)

[242]:
```
from sklearn.decomposition import PCA
# PCA function from the decomposition package is used to identify the Principal␣
 ↪Component that provides the best variance in the output.
pca = PCA(n_components=13)
# In our case we are identifying the first two principal attributes
wine_std_pca = pca.fit_transform(wine_std.iloc[:,0:13])
pca.explained_variance_ratio_

# From the above we can see that the first two components in itself accounts␣
 ↪for almost 56% of variance.
# Hence we will use only two components for our k-mean clustering algorithm
```

[242]:
```
array([0.36198848, 0.1920749 , 0.11123631, 0.0706903 , 0.06563294,
       0.04935823, 0.04238679, 0.02680749, 0.02222153, 0.01930019,
       0.01736836, 0.01298233, 0.00795215])
```

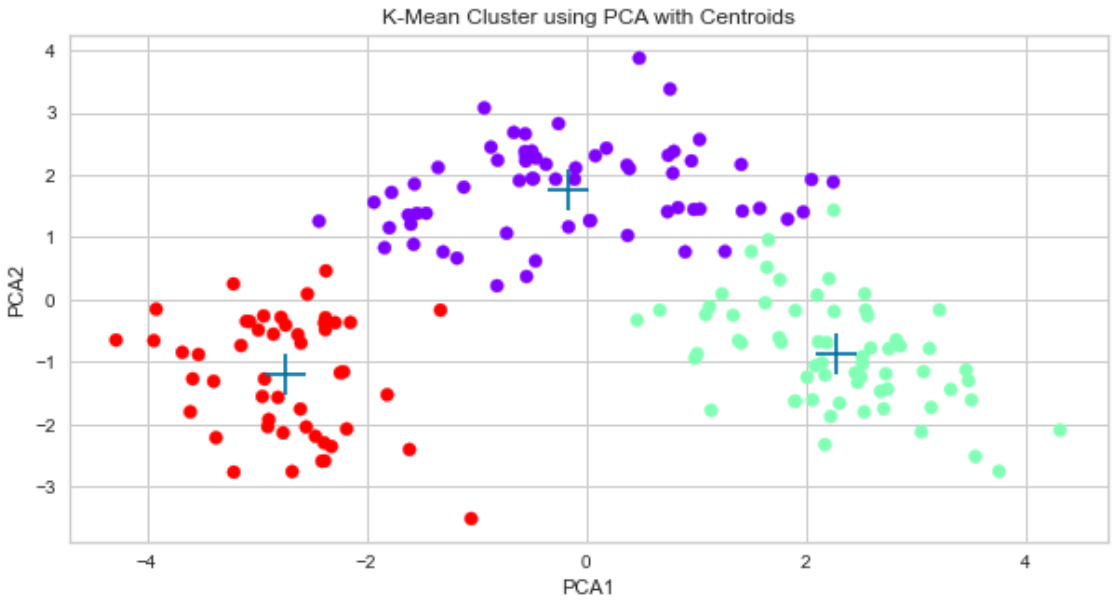
[251]:
```
# Select the first two principal components as input for the kmean
win_std_pca_in = pd.DataFrame(wine_std_pca, columns =␣
 ↪['PCA1','PCA2','PCA3','PCA4', 'PCA5',␣
 ↪'PCA6','PCA7','PCA8','PCA9','PCA10','PCA11','PCA12','PCA13'])
X_PCA = win_std_pca_in.iloc[:,0:2]
```

[255]:
```
# Let us re-run the kmean algorithm withe selected PCA component
km_PCA = KMeans(n_clusters=3,max_iter=300)
y_km_PCA = km_PCA.fit_predict(X_PCA)

wine_std['Pred_Type_PCA'] = y_km_PCA
kmc_PCA=km_PCA.cluster_centers_
```

Let us plot the resulted k-mean cluster created using the PCA component and see how the new clustering looks compared to the older one.

[260]:
```
fig, (ax0) = plt.subplots(1, figsize=(10, 5))
ax0.set_title('K-Mean Cluster using PCA with Centroids')
ax0.scatter(X_PCA['PCA1'],X_PCA['PCA2'], c=y_km_PCA, cmap='rainbow')
ax0.scatter(kmc_PCA[:,0],kmc_PCA[:,1],  marker="+", s=500, c='b')
plt.xlabel('PCA1')
plt.ylabel('PCA2')
plt.show()
```



From above we can very well see that the cluster boundaries are more prominent with almost no overlapping of the datapoints.

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